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2-Propanol (67-63-0)[1]

2. Physico-chemical Properties

2.1 Melting Point

Value	= - 90 degree C
Decomposition	
Sublimation	
Method	other
Year	
GLP	no
Test condition	Method is ASTM D 97
Reference	Shell Chemicals data sheet IS 3.2.4 dated June 1992

2.2 Boiling Point

Value	ca. 82 - 83 degree C
Pressure	1012 hPa
Decomposition	no
Method	other
Year	
GLP	no
Test condition	ASTM D 1 078, standard method for distillation range
Reference	Shell Chemicals data sheet IS 3.2.4 dated June 1992

2.3 Density

Type	density
Value	ca. 0.785 - 0.786 g/cm3
Temperature	20 degree C
Method	other
Year	
GLP	no
Test condition	ASTM D4052, Standard method for density
Reference	Shell Chemicals data sheet IS 3.2.4 dated June 1992

2.4 Vapour Pressure

[1] All summaries, except section 3.3.2 Stability in Soil, are from the 2-Propanol OECD SIDS document.

Value	= 43 hPa
Temperature	20 degree C
Method	other
Year	
GLP	
Reference	Shell Chemicals data sheet IS 3.2.4 dated June 1992

2.5 Partition Coefficient

log Pow	=0.05
Temperature	25 degree C
Method	other (measured)
Year	1973
GLP	no
Reference	data Dillingham, E.O. et aI., IPharm.Sci., 62, 1973,22. In Pomona Data File on Log P and related parameters.

2.6.1 Water Solubility

Value	= 100 vol% at 20 degree C
pH	Concentration at degree C
pKa	at 25 degree C
Descr.	miscible
Method	other
Year	
GLP	
Reference	Shell Chemicals Data sheet IS 3.2.4 dated June 1992

2.7 Flash Point

Value	= 12 degrees C
Type	closed cup
Method	other
Year	
GLP	no
Test condition	IP 170, Standard method for flash point
Reference	Shell Chemicals data sheet IS 3.2.4 dated June 1992

2.8 Autoflammability

Value	= 425 degree C
Pressure	
Method	other
Year	
GLP	no
Test condition	ASTM D2155, Standard method for autoignition

Reference Shell Chemicals data sheet IS 3.2.4 dated June 1992

2.12 Viscosity

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3. Environmental Fate and Pathways

3.1 Photodegradation

Type air
Light Source Sun light
Light Spect. ca. 290 - 900 nm
ReI. Intens. = 100 based on Intensity of Sunlight
Spectrun of Substance lambda (max) [>295nm] nm epsilon (max) epsilon (295)

Conc. of Substance Temperature _____degree C_____

Direct Photolysis
Halflife tl/2
Degradation % after
Quantum yield

Indirect Photolysis
Type air
Indirect photolysis
Sensitizer NO3
Rate Constant <= .0000000000000023 cm3/(molecule*sec)
Method other (measured): Flash- Photolysis- Visible Absorption
Year 1987
GLP no data
Test substance other TS: >= 99% pure
Remark Estimated troposphere half-life of 2-propanol for a "clean" troposphere with 10 ppt (approximately 2.4* l0E8 radicals/cm3 of NO3 radicals during night-time hours, tl/2 >= 14.5 d.
Test condition 25 degrees C, total pressure of 133.3 hPa of NO2 diluent
Reference Wallington, TJ. et al. (1987): Int J Chem Kinet 19, 243-249.

Type air
Indirect photolysis
Sensitizer OH
Rate constant = .0000000000051 cm3/(molecule*sec)
Method OECD Guide-line draft "Photochemical Oxidative Degradation in the
Year 1987

GLP	no data
Test Substance	no data
Remark	Estimated troposheric half-life of 2-propanol with an average tropospheric OH radical concentration of 5*I0E5 radicals/cm3, t1/2 = 3.1 d.
Test condition	smog-chamber: 27 degrees C, 0.105 - 0.110 Mpa, UV-A lamps (1.5 m long, 65 W Hg low pressure lamps, TL 65-80 W/05), maximum volume-averaged UV intensity (k1 of NO2 photolysis amounted to about k1 = 0.9 min-l) corresponding to twice the solar UV intensity at sea level and midlatitudes, OH source: HONO photolysis.
Reference	Kloepffer, W. et al. (1988): Ecotoxicol Environ Safety 15,298-319.

Type	air
Indirect photolysis	
Sensitizer	OH
Rate constant	= .00000000000521 cm3/(molecule*sec)
Method	other (measured): Photodegradation by Indirect Photolysis 1990
Year	
GLP	no data
Test substance	no data
Remark	Estimated tropospheric half-life of 2-propanol, with an OH radical concentration of 5*10E5 radicals/cm3, t1/2 = 3.1 d.
Test condition	25 degrees C
Reference	Atkinson, R. (1990): J Phys Chern Ref Data (1992),21(6):1125-1568

Type	air
Indirect photolysis	
Sensitizer	OH
Conc. of Sensitizer	500000 molecules/cm3
Rate constant	= .00000000000521 cm3/(molecule*sec)
Degradation	= 50% after 6.2 days
Method	other (measured): AOP Computer Program, Vers. 1.53, Syracuse Research Center (based upon reference).
Year	1994
GLP	no data
Test substance	no data
Remark	Half-life refers to 12 hour-days Atkinson, R.: A structure-activity relationship for the estimation of rate constants for the gas-phase reactions of OH radicals with organic compounds.
Reference	Int J Chem Kinet 19, 799-828 (1987)

Type	air
Indirect photolysis	
Sensitizer	OH
Rate constant	= .00000000000532 cm^3/(molecule*sec)

Method	other (calculated): Prediction of the OH reaction rate constant by correlation of the negative logarithm of OH reaction rate constants with the first vertical ionisation energy of organic compounds in the gas phase.
Year	1984
GLP	no data
Test substance	no data
Remark	The correlation of the negative logarithm of OH reaction rate constants with the first vertical ionization energy of organic compounds in the gas phase enables the prediction of kOH with a probability of about 90%; estimated tropospheric half-life of 2 propanol, assessing a global diurnal mean of OH radical concentration of 5*10E5 radicals/cm3, t1/2 = 3.0 d.
Test condition	27 degrees C
Reference	Guesten, H. et al. (1984): J Atmos Chern 2,83-93.
Type	air
Indirect photolysis	
Sensitizer	OH
Rate constant	= .00000000000548 cm3/(mo1ecule*sec)
Method	other (measured): Flash-Photolysis Resonance-Asorption Technique
Year	1978
GLP	no data
Test substance	no data
Remark	Estimated tropospheric half-life of 2 propanol, with an OH radical concentration of 5* 10E5 radicals/cm3, tl/2 = 2.9 d.
Test condition	23 degrees C, 200 hPa
Reference	Overend, R., Paraskevopou1os, G. (1978): J Phys Chern 82, 13291333.
Type	air
Indirect photolysis	
Sensitizer	OH
Rate constant	= .0000000000062 cm3/(molecule*sec)
Method	other (measured): Photodegradation by Indirect Photolysis
Year	1985
GLP	no data
Test substance	no data
Remark	Estimated tropospheric half-life of 2-propanol, with an OH radical concentration of 5*l0E5 radicals/cm3, t1/2 = 2.6 d.
Test condition	room temperature
Reference	Atkinson, R. (1985): Chern Rev 85, pp. 69-75, 135-153, 182-201.

Type	air
Indirect photolysis	
Sensitizer	OH
Rate constant	= .0000000000071 cm3/(molecule*sec)
Method	other (measured): Environmental Chamber Photo oxidation Study
Year	1976
GLP	no data
Test substance	no data
Remark	Estimated atmospheric half-life of 2-propanol, with an average ambient OH radical concentration of 5/l0E6 radicals/cm3, tl/2 - 5.4 h.
Test condition	Smog-chamber: ca. 32 degrees C, 1013 hPa, OH source: HONO photolysis and the reaction ofNO2 with NO.
Reference	Lloyd, A.c. et al. (1976): Chern Phys Lett. 42, 205-209.

3.1.2 Stability in Water

Type	abiotic
Remark	Propan-2-ol is not susceptible to hydrolysis.
Reference	P.H. Howard, Handbook of Environmental Fate and Exposure Data for OrganicChemicals, Lewis Publishers Inc., Chelsea Michigan USA, 1990, p.304 -309.
Type	biotic
tI/2 pH4	
tI/2 pH7	= 5 days at 20 degree C
tl/2 pH9	
tl/2 pH	
Degradation pH 7	at 20 degree C: = 50 % after 5 days
Method	other
Year	1979
GLP	no data
Test substance	as prescribed by 1.1 - 1.4
Test condition	APHA-219 (1971) at 20 degree C.
Reference	Bridie, A.L., Wolff, C.J.M. & Winter, M., Water Research, 13, 1979, 627 - 630.

3.3.1 Distribution

Media	air - biota - sediment(s) - soil - water
Method	Calculation according Mackay, Level I
Year	1981
Result	Air 22.3 %m;

	Water 77.7 %m; Soil 0.0 %m; Sediment 0.0 %m; Biota 0.0 %m.
Reference	Mackay, D. & Paterson, S., Calculating Fugacity, Environm. Sci. Technol., 15(9), 1981, 1006 -10 14.

3.3.2 Stability in Soil

Media	other
Method	Calculation according to PCKOCWIN v1.66 Results
Year	2006
Result	First Order Molecular Connectivity Index: 1.732 Non-Corrected Log Koc: 1.5445 Fragment Correction(s): 1 Aliphatic Alcohol (-C-OH): -1.5193 Corrected Log Koc: 0.0252 Estimated Koc: 1.06
Reliability	(2) valid with restrictions The value was predicted using accepted calculation methods.
Reference	USEPA, EPISUITE v3.12, 2006.

3.5 Biodegradation

Type	aerobic
Inoculum	predominantly domestic sewage, non-adapted
Concentration	1.5 mg/1 related to Test substance
Degradation	= 49 % after 5 day
Results	readily biodegradable
Kinetic	
Method	other
Year	1979
GLP	no data
Test substance	> 99.7% (w/w) 2-propanol
Test condition	APHA-219 (1971) at 20 degree C.
Reference	A) Bridie, A.L., Wolff, C.J.M., & Winter, M. BOD and COD of some Petrochemicals, Water Research, 13, 1979, p. 627 -630. B) Idem, Shell Group Research Report, AMGR.0224.74

Type	aerobic
Inoculum	domestic sewage, non-adapted
Concentration	3, 7 and 10 mg/1 related to Test substance
Degradation	= 77 % after 10 day
Results	readily biodegradable

Kinetic	5 day = 28 10 day = 77 15 day = 80 20 day = 78
Method	other
Year	1974
GLP	no data
Test substance	> 99.7% (w/w) 2-propanol
Test condition	As described in reference.
Reference	Price, K.S. Waggy, G.T. & Conway, R.A., Brine Shrimp Bioassay and Seawater BOD of Petrochemicals, J. Water Pol1ut. Contr. Fed., 46.1974,63 - 77.

Type	aerobic
Inoculum	domestic sewage, non-adapted
Concentration	3, 7 and 10 mg/1 related to Test substance
Degradation	= 42 % after 10 day
Results	
Kinetic	5 day = 13 10day= 42 15 day = 60 20 day = 72
Method	other
Year	1974
GLP	no data
Test substance	> 99.7% (w/w) 2-propanol
Test condition	As described in reference. The test medium is artificial seawater.
Reference	Price, K.S., Waggy, G.T. & Conway, R.A., Brine Shrimp Bioassay and Seawater BOD of Petrochemicals, J. Water Pollut. Contr. Fed., 46, 1974,63 - 77.

4. Ecotoxicity

4.1 Acute/Prolonged Toxicity to Fish

Type	flow through
Species	*Pimephales promelas*
Unit	mg/l
Exposure Period	96 hour
NOEC	
LC0	
LC50	= 9640
LC100	
Analyt. Monitoring	yes
Method	other
Year	1983

GLP	no data
Test substance	> 99.7% (w/w) 2-propanol
Test condition	As described in reference.
Reference	Veith, G.D., Call, DJ. & Brooke, L.T., Estimating the Acute Toxicity of Narcotic Industrial Chemicals to Fathead Minnows. In: Bishop, W.E., Cardwell, R.D. & Heidolph, B.B. Eds. Aquatic Toxicology and Hazard Assessment: 6th Symp., ASTM STP 802, Philadelphia (USA), 1983,90 - 97.

4.2 Acute Toxicity to Daphnia

Species	*Daphnia magna*
Unit	mg/l
Exposure Period	24 hour
NOEC	
EC0	
EC50	> 10000
EC100	
Analyt. Monitoring	no
Method	other
Year	1977
GLP	no data
Test Substance	> 99.7% (w/w) 2-propanol
Test condition	As described in reference.
Reference	Bringmann, G. & Kuehn, R., Results of the Damaging Effect of Water Pollutants on Daphnia magna, Z. Wasser Abwasser Forsch., 10(5), 1977, 161 - 166.

Species	*Crangon crangon*
Unit	mg/l
Exposure Period	48 hour
NOEC	
EC0	
EC50	
EC100	
LC50	= 1400
Analyt. Monitoring	no
Method	other
Year	1974
GLP	no data
Test Substance	> 99.7% (w/w) 2-propanol
Remark	The species is a marine invertebrate.
Test condition	As described in reference. Renewal.
Reference	Blackman, R.A.A., Toxicity of Oil-Sinking Agents, Mar. Po1lut. Bull., 5, 1974, 116 - 118.

4.3 Toxicity to Aquatic Plants (e.g. algae)

Species	Scenedesmus quadricauda
Endpoint	growth rate
Unit	mg/L
Exposure Period	7 day
NOEC	
LOEC	
EC0	
EC10	
EC50	
Analyt. Monitoring	no
Method	other
Year	1980
GLP	no data
Test substance	> 99.7% (w/w) 2-propanol
Test condition	As described in reference.
Remark	Toxicity threshold concentration = 1800 mg/L.
Reference	Bringmann, G. & Kuehn, R., Comparison of the Toxicity Thresholds of Water Pollutants to Bacteria, Algae and Protozoa in the Cell Multiplication Inhibition Test, Water Research, 14, 1980,231 - 241.

4.5.2 Chronic Toxicity to Daphnia

Species	Daphnia magna (Crustacea)
Exposure period	16 day
Unit	mg/L
Analyt. monitoring	yes
NOEC	= 141
Method	other: Prolonged Toxicity Test
Year	1985
GLP	no data
Test substance	no data
Remark	NOEC on growth: highest concentration which did not result in a significant reduction in growth at $p < 0.001$.
Reference	Hermens, J. et al (1985): Aquatic Toxicol. 6, 209-217.

Species	Daphnia magna (Crustacea)
Exposure period	21 day
Unit	mg/L
Analyt. Monitoring	no
NOEC	=30
EC50	> 100
EC29	= 100

Method	other: UBA- Verfahrensvorschlag: Verlaengerter Toxizitaetstest bei Daphnia magna
Year	1984
GLP	no
Test Substance	> 99.7% (w/w) 2-propanol
Reference	Huel-Bericht DL 106, 1988 (unveroeffentlicht)

5. Toxicity

5.1.1 Acute Oral Toxicity

Type	LD50
Species	rat
Value	= 5280 mg/kg
Method	other
Year	1944
GLP	no
Test substance	> 99.7% (w/w) 2-propanol
Reference	Lehman, A. J., Chase, H.F., (1944) 1. Lab. C1in. Med. 29: 561 - 567.

Type	LD50
Species	rat
Value	= 5840 mg/kg
Method	other
Year	1948
GLP	no
Test substance	> 99.7% (w/w) 2-propanol
Reference	Smyth, H.F., Carpenter, C.P., (1948), 1. Ind. Hyg. Toxicol.,30: 63-70.

Type	LD50
Species	rat
Value	= 4710 mg/kg
Method	other
Year	1971
GLP	no
Test substance	> 99.7% (w/w) 2-propanol
Remark	Three LD50 values presented: 5.6, 6.0 and 6.8 mllkg for neonates, young adult and old rats respectively. Quoted value is a mean of the three as presented in IPCS ERC document on 2-propanol (1990).
Reference	Kimura, E.T., Ebert, D.M., Dodge, P.W., (1971), Toxicol. Appl. Pharmacal., 19: 699 -703.

Type	LD50
Species	Rat

Value	= 5500 mg/kg
Method	other
Year	1985
GLP	no
Test substance	> 99.7% (w/w) 2-propanol
Reference	Guseinov, V.G., (1985), Gig. Tr. Prof. Zabol. (7): 60-62.

Type	LD50
Species	mouse
Value	= 4475 mg/kg
Method	other
Year	1985
GLP	no
Test substance	> 99.7% (w/w) 2-propanol
Reference	Guseinov, Y.G., (1985), Gig. Tr. Prof Zabol., (7): 60-62.

Type	LD50
Species	rabbit
Value	= 5030 mg/kg
Method	other
Year	1944
GLP	no
Test substance	> 99.7% (w/w) 2-propanol
Reference	Lehman, AJ., Chase, H.F. (1944),1. Lab. CIin. Med., 29: 561 - 567.

Type	LD50
Species	rabbit
Value	= 7990 mg/kg
Method	other
Year	1972
GLP	no
Test substance	> 99.7% (w/w) 2-propanol
Reference	Munch, le., (1972), Ind. Med. 41: 31 - 33.

5.1.2 Acute Inhalation Toxicity

Type	LC50
Species	rat
Exposure Time	4 hour
Value	= 72.6 mg/l
Method	other
Year	1985
GLP	no
Test Substance	> 99.7% (w/w) 2-propanol
Reference	Guseinov, Y.G., (1985), Gig. Tr. Prof Zabol. (7): 60 - 62.

Type	LC50
Species	rat
Exposure Time	8 hour
Value	= 51.045 mg/L
Method	other
Year	1979
GLP	no
Test Substance	> 99.7% (w/w) 2-propanol
Reference	Laham, S., Potvin, M., Schrader, K., Marino, I. (1979), Drug. Chern. Toxicol. 3: 343 -360.

Type	LC50
Species	mouse
Exposure Time	2 hour
Value	= 53 mg/L
Method	other 1
Year	985
GLP	no
Test Substance	> 99.7% (w/w) 2-propanol
Reference	Guseinov, v.G., (1985), Gig. Tr. Prof. Zabol, (7), 60-62.

5.1.3 Acute Dermal Toxicity

Type	LD50
Species	rabbit
Value	= 12870 mg/kg
Method	other
Year	1948
GLP	no
Test Substance	> 99.7% (w/w) 2-propanol
Reference	Smyth, H.F., Carpenter, c.P., (1948), J. Ind. Hyg. Toxicol.,30: 63 -70.

5.2.1 Skin Irritation

Species	rabbit
Result	not irritating
Classification	not irritating
Method	other
Year	1975
GLP	no
Test Substance	> 99.7% (w/w) 2-propanol
Reference	Nixon, G.A., Tyson, CA., Wertz, w.e., (1975), Toxicol. Appl. Pharmacal. 31: 481 -490.

5.2.2 Eye Irritation

Species	rabbit
Result	irritating
Classification	irritating
Method	Draize- Test
Year	1973
GLP	no
Test substance	> 99.7% (w/w) 2-propanol
Reference	Marzulli, F.N., Ruggles, D.L, (1973), J. P£soc. Off. Anal. Chern., 56: 905 - 914.

Species	rabbit
Result	moderately irritating
Classification	irritating
Method	Draize- Test
Year	1980
GLP	no
Test substance	> 99.7% (w/w) 2-propanol
Reference	Griffith, IF., Nixon, GA, Bruce, R.D., Reer, PJ., Bannan, E.A., (1980), Toxicol. Appl. Pharmacol. 55: 501 - 513.

Species	rabbit
Result	irritating
Classification	R36
Method	Draize- Test
Year	1986
GLP	Yes
Test substance	> 99.7% (w/w) 2-propanol
Reference	Exxon Biomedical Sciences Inc. (1986) Ocular Irritation Study in Rabbits (Isopropanol). EBSI Document No. 86MRL272.

Species	rabbit
Result	moderate irritating
Classification	irritating
Method	Draize- Test
Year	1987
GLP	no data
Test substance	> 99.7% (w/w) 2-propanol
Remark	Study gives maximum Draize score of 37 (out of 110) and provided conflicting data from 2 tests, one moderate and the other severely irritating.
Reference	Morgan, R.L., Sorenson, S.S., Castles, T.R., (1987), Food. Chem. Toxicol., 25: 609 -613.

5.3 Sensitization

Type	Buehler-Test
Species	Guinea pig
Result	not sensitizing
Classification	not sensitizing
Method	other
Year	1980
GLP	no
Test substance	> 99.7% (w/w) 2-propanol
Remark	Result given as "No sensitisation (0/20)". No other data on sensitisation have been found.
Reference	P & G, Unpublished data.

5.4 Repeated Dose Toxicity

Species	rat
Strain	Fischer 344
Sex	male/female
Route of Administration	inhalation
Exposure Period	13 weeks
Frequency of Treatment	6 hours/day, 5 days/week
Post Exposure Observ. Period	none
Doses	0, 100,500, 1500 and 5000 ppm
Control Group	yes
NOEL	500
LOEL	1500
Method	other (US EPA TCSA Test Guidelines)
Year	1994
GLP	yes
Test Substance	> 99.7% (w/w) 2-propanol
Remark	No exposure-related mortalities occurred. Narcotic effects were noted during exposures to 1500 and 5000 ppm. Ataxia was observed following exposure to 5000 ppm. Decreases in body weight were also observed at the end of the first week of exposure to 5000 ppm. The only microscopic change observed was hyaline droplets within the kidneys of all male rats (including controls). The size and frequency of these droplets were increased in the exposed groups. Thus, repeated exposures produced toxic effects only at the highest concentration (5000 ppm) and a kidney change in male rats of unknown biological significance.
Reference	Burleigh-Flayer, H.D., et al. (1994). Fundam. Appl. Toxicol. 23, 421428.

Species	rat
Strain	Wistar

Sex	male
Route of Administration	inhalation
Exposure Period	13 or 20 weeks
Frequency of Treatment	4 hours/day, 5 days/week.
Post Exposure Observ. Period	none
Doses	400, 1000,4000, 8000 ppm for 12 weeks; 1000 and 8000 ppm for 20 weeks
Control Group	yes
NOEL	= 400 ppm
LOEL	= 1000 ppm
Method	other
Year	1991
GLP	no data
Test Substance	> 99.7% (w/w) 2-propanol
Remark	No significant differences appeared between the groups exposed to 400 ppm and the control group in body weight and in hematological and serum chemistry tests. There was inhibition of body weight and marked local irritation in groups given 1000 ppm or more, decrease in erythrocyte and hemoglobin values in groups given 4000 ppm or more, and increases in serum GOT and GPT, and total cholesterol in the 8000 ppm group. Nakaseko et al. also exposed rats to 1000 and 8000 ppm isopropanol for 20 weeks for nerve conduction studies, which was reported separately (see also section 5.10).
Reference	Nakaseko, H., Teramoto, K., Horiguchi, S., Wakitani, F., Yamanoto, T., Adachi, M., Tanaka, H., Hozu, S., lpn. 1. Ind.Hlth. 33(3): 200201, 1991.

Species	rat
Strain	F-344
Sex	female
Route of Administration	Inhalation
Exposure Period	90 days or 63 days
Frequency of Treatment	1/2 6 hours/day for 5 days /week for 13 weeks
Post Exposure Observ. Period	1/2 6 hours/ day for 5 days /week for 9 weeks 2 weeks post exposure
Doses	5000 ppm
Control Group	yes
NOEL	NA
LOEL	5000 ppm
Method	other
Year	1994
GLP	yes
Test Substance	> 99.7% (w/w) 2-propanol
Remark	Increases in motor activity were seen following exposure to 5000 ppm of isopropanol. After 9 weeks of exposure, complete recovery

	was noted two days post exposure. After 13 weeks of exposure, complete reversibility was noted at 2 weeks post exposure.
Reference	Gill, M., Burleigh-Flayer, H., Bevan. C., Gardiner, T., Kapp, R., Isopropanol Ninety-Day Vapor Inhalation Neurotoxicity Study in Female F-344 Rats. (Abstract) The Toxicologist, Vol. 14 (1), 1994.
Species	rat
Strain	no data
Sex	male/female
Route of Administration	drinking water
Exposure Period	27 weeks
Frequency of Treatment	continuous
Post Exposure Observ. Period	none
Doses	600 & 2300 mg/kg for males, 1000 & 3900 mg/kg for females
Control Group	yes
NOEL	= 600 - 1000 mg/kg bw d
LOEL	= 2300 - 3900 mg/kg bw d
Method	other
Year	1944
GLP	no
Test Substance	> 99.7% (w/w) 2-propanol
Remark	The male rats showed some decreased body weight gains during the first thirteen weeks of the study, and then increased body weight gain for the reminder of the study. The female rats showed decreased body weight gain throughout the study. No gross or microscopic abnormalities were noted.
Reference	Lehman, A.J., Chase, H.F., (1944), J. Lab. Clin. Med. 29: 561 - 567.
Species	rat
Strain	no data
Sex	male
Route of Administration	drinking water
Exposure Period	12 weeks
Frequency of Treatment	continuous
Post Exposure Observ. Period	none
Doses	1, 2, 3 and 5 percent
Control Group	yes
NOEL	= 1 % (870 mg/kg/day)
LOEL	= 2% (1280 mg/kg/day)
Method	other
Year	1993
GLP	no data
Test Substance	> 99.7% (w/w) 2-propanol
Remark	The relative organ weights of liver, kidneys, and adrenals were

	significantly increased in a dose dependent manner. No histological alterations could be attributed to the dosing, apart from a dose dependent increase in formation of hyaline casts and droplets in the proximal tubules of the kidneys. Dorsal hippocampal glial fibrillary acidic protein (GF AP) was unaffected after treatment.
Reference	Pilegaard, K. and Ladefoged, O. (1993) In Vivo 7:325-330
Species	mouse
Strain	CD-l
Sex	male/female
Route of Administration	inhalation
Exposure Period	13 weeks
Frequency of Treatment	6 hours/day, 5 days/week
Post Exposure Observ. Period	none
Doses	0, 100, 500, 1500 and 5000 ppm
Control Group	yes
NOEL	= 500 ppm
LOEL	= 1500 ppm
Method	other (US BPA TCSA Test Guidelines)
Year	1994
GLP	> 99.7% (w/w) 2-propanol
Test Substance	No exposure-related mortalities occurred. Narcotic effects were noted
Remark	during exposures to 1500 and 5000 ppm. No exposure-related effects were noted on body weight of the male mice, but increased body weight and body weight gain were observed for the 5000 ppm female mice. No treatmentrelated effects were noted at gross necropsy or at histopathologic examination.
Reference	Burleigh-Flayer, H.D., et al. (1994). Fundam. Appl. Toxicol. 23, 421428.
Species	rat
Strain	Fischer 344
Sex	male/female
Route of Administration	inhalation
Exposure Period	13 weeks
Frequency of Treatment	6 hours/day, 5 days/week
Post Exposure Observ. Period	none
Doses	0, 500, 1500 and 5000 ppm
Control Group	yes
NOEL	= 1500
LOEL	= 5000
Method	other (US EPA TCSA Test Guidelines)
Year	1994
GLP	yes
Test Substance	> 99.7% (w/w) 2-propanol

Remark	Neurobehavioral evaluations included a functional observation battery (FOB), motor activity, and neuropathology. There were no changes in FOB, but increased motor activity was noted in female rats of the 5000 ppm group at week 9 and 13. Neuropathological examination revealed no exposure-related lesions in the nervous system.
Reference	Burleigh-Player, H.D., et al. (1994). Fundam. Appl. Toxicol. 23, 421428.

5.5 Genetic Toxicity in Vitro

Type	Salmonella typhimurium reverse mutation assay
System of Testing	TA 98, 100, 1535, 1537
Concentr.	180 mmol/plate
Metabolic Activation	with and without
Result	negative
Method	other
Year	1980
GLP	no data
Test substance	> 99.7% (w/w) 2-propanol
Remark	A report on screening of many chemicals which could be constituents of tobacco smoke.
Reference	Florin, 1, Rutberg, L., Curvall, M., and Enzell, OR Toxicology 15:219-232, 1980

Type	Sister chromatid exchange assay
System of Testing	Chinese hamster V79 fibroblasts
Concentr.	3.3, 10,33.3 and 100 mmol/l
Metabolic Activation	with and without
Result	negative
Method	other
Year	1987
GLP	no data
Test substance	> 99.7% (w/w) 2-propanol
Reference	Von der Hude, W., Scheutwinkel, M., Gramlich, u., Fissler, B., Busler, A., In Vitro Environ. Mutagen., (1987), 9: 401 - 410.

Type	Salmonella typhimurium reverse mutation assay
System of Testing	TA 97, 98, 100, 102, 104, 1535, 1537, 1538
Concentr.	100 mmol/plate
Metabolic Activation	with and without
Result	negative
Method	other
Year	1992
GLP	Yes

Test substance	> 99.7% (w/w) 2-propanol
Reference	Zeiger,E.etal,Env.Mo1.Mut., 19(5upp1.21):2-141, 1992.

Type	Meiotic nondisjunction
System of Testing	Neurospora crassa (Strain I x I)
Concentr.	no data
Metabolic Activation	without
Result	negative
Method	other
Year	1980
GLP	no data
Test substance	> 99.7% (w/w) 2-propanol
Reference	Griffiths AlF. (1980). NIEHS 263-77-C0604CC, Progress Report. (Cited In: Brockman RE., de Serres FJ., Ong T-M., DeMarini D.M., Katz Al, Griffiths AlF. and Stafford R.S. (1984). Mutation tests in Neurospora crassa. A report of the U.S. Environmental Protection Agency Gene- Tox Program. Mutat. Res. 133:87-134.)

Type	Cell transformation
System of Testing	SA 7/Syrian Hamster Embryo
Concentr.	62 - 1000 µg/ml
Metabolic Activation	without
Result	negative
Method	other
Year	1978
GLP	no data
Test substance	> 99.7% (w/w) 2-propanol
Reference	Casto B.C. and Hatch G.G. (1978). Progress Report NIH-NCI-N01CP-45615. pp. 62-75. (Cited In: Heidelberger C., Freeman A.E., Pienta R.I., Sivak A., Bertram lS., Casto B.c., Dunkel V.C., Francis M.W., Kakunaga T., Little lB. and Schechtman L.M. (1983). Cell transformation by chemical agents - a review and analysis of the literature. A report of the U.S. Environmental Protection Agency Gene- Tox Progranl. Mutat. Res. 114:283-385.)

5.6 Genetic Toxicity in Vivo

Type	Micronucleus Assay
Species	Mouse
Strain	ICR random bred
Sex	male/female
Route of Administration	i.p.
Exposure Period	once, bone marrow examined after 24, 48 and 72 hours.
Doses	350, 1173, 2500 mg/kg
Result	negative

Method	other (US EPA TCSA Test Guidelines)
Year	1993
GLP	yes
Test Substance	> 99.7% (w/w) 2-propanol
Reference	Kapp, R.W. et al. (1993). Environ. Mol. Mutagen., 22: 93-100.

5.8.1 Toxicity to Reproduction

Type	One generation study
Species	rat
Strain	Wistar
Sex	male/female
Route of Administration	drinking water
Exposure Period	To weaning (day 21 after birth).
Frequency of Treatment	continuous
Premating Exposure Period	
male	70 days
female	21 days
Duration of Test	To weaning
Doses	0.5, 1.0 and 2.0%
Control Group	yes
NOEL Parental	= 1 %
NOEL FI Offspring	= 1 %
NOEL F2 Offspring	
Method	other
Year	1986
GLP	yes
Test Substance	> 99.7% (w/w) 2-propanol
Remark	Parental rats dosed with 2% isopropanol had decreased body weight gain and corresponding reduced pup weight gain and decreased survival compared with controls. There was also a dose-related increase in relative liver weights of the F 1 animals. There was no effect on reproductive parameters. There was no macroscopic or histopathological changes associated with isopropanol treatment. The reproductive NOEL of 1 % corresponds to 825 and 625 mg/kg/day for females and males respectively. A further study by Lehman et al (J. Exp. Pharmacol. Expt. Therapy, 85, 61-69, 1945) studied the effects of IP A in drinking water. No effects were found at 2.5% but the reported data are scant.
Reference	British Industrial Biological Research Assoc., Report 0570/3/86.

Type	Two generation study
Species	rat
Strain	Sprague- Dawley
Sex	male/female

Route of Administration	gavage
Exposure Period	Prior to mating and to lactation and weaning of F 1 and F2 generations.
Frequency of Treatment	daily
Premating Exposure Period	
male	10 weeks
female	10 weeks
Duration of Test	to lactation and weaning
Doses	100,500 and 1000 mg/kg/day
Control Group	yes
NOEL Parental	< 500 mglkg bw/day (BMDLl0 = 407 mglkg/day)(see remarks below)
NOEL FI Offspring	< 500 mglkg bw/day(BMDL5 = 449 mglkg/day)(See remarks below)
NOEL F2 Offspring	< 500 mglkg bw/day (BMDL5 = 418 mg/kg/day)(See remarks below)
Method	other (US EPA TCSA Test Guidelines)
Year	1995
GLP	yes
Test Substance	> 99.7% (w/w) 2-propanol
Remark	Thirty rats of each sex per group (PI) were dosed once daily by oral gavage with 0, 100, 500 or 1000 mg of isopropanol kg-l Dr at least 10 weeks prior to mating. Findings in the parental animals included increased lactation body weight gain in the 500 and 1000 mg/kg females, increased liver and kidney weights in the 500 and 1000 mg/kg groups of both sexes, and centrilobular hepatocyte hyperthrophy in some P2 males. There was microscopic findings in the kidneys from the mid- and high-dose PI males and from all treated groups of the P2 males. Exposure to 1000 mg/kg day and to a lesser extent 500 mg/kg day resulted in a reduction in postnatal survival in both Fl and F2 litters. In addition, offspring body weight was reduced during the early postnatal period in the 1000 mg/kg Fl males and in the 1000 mg/kg F2 pups of both sexes. In the 1000 mg/kg group 18/70 Fl weanlings or were euthanized prior to P2 selection. No treatment-related postmortem findings were observed in the offspring from either generation. A statistically significant reduction was observed in the male mating index of the 1000 mg/kg P2 males compared to controls. However, no treatment-related microscopic changes in reproductive tissues or biologically meaningful differences in other reproductive parameters were noted. The study-derived NOELs for the Fl and F2 offspring are contingent upon the biological significance ascribed to the effects observed for the 500 mg/kg /day treatment group. There are two perspectives on the interpretation of these observations. A conservative perspective is that the reductions in postnatal survival are treatment- and dose related effects (U.S. EPA, 1992 U.S. EPA, 1996; Tyl, 1996). Consequently, the NOEL based on this interpretation would be set at

100 mg/kg/day. On the other hand, the NOEL may be set at 500 mg/kg/day if these observations are not deemed biologically significant (Bevan et al., 1995; Harris, 1995). A benchmark dose (BMD) assessment was conducted as a way of clarifying issues surrounding the derivation of effect levels for this study. As described below, this assessment resulted in calculated BMD dosages of 449 and 418 mg/kg low/day for the Fl and F2, respectively as appropriate descriptors for this endpoint. (See Benchmark study below.).

Reference

Bevan, c., Tyler, T.R., Gardiner, T.R., Kapp, R.W., Jr., Andrews, L. and Beyer, B.K. Journal of Applied Toxicology, Vol. 15(2) pp. 117123 (1995).

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US EPA, Draft Final RM1 Risk Assessment of Isopropanol, OPPT, 1996. TSCA Public Docket Number AR-141.

Quantitative Dose-Rsponse Analysis -- Application of the Benchmark Method to the Multi-Generation Rat Reproduction Study for Isopropanol.

Chemical Manufacturers Association Isopropanol Panel conducted a quantitative dose-response analysis of the bioassay data from the multi- generation rat reproduction study noted above using the benchmark dose method to identifY the relevant dosage to derive a toxicity value that may contribute in part to safety assessment decisions for isopropanol.

The reproductive/developmental effects were reported to have NOAEL between 100 mg/kg/day (USEPA 1992) and 500 mg/kg/day (Bevan et aI., 1995). Based upon decrease in mating index observed in the P2 males, a BMDLl0 of 407 mg/kg/day was estimated for reproductive effects. A BMDL5 of 418 mg/kg/day was estimated for developmental effects based upon the F2 generation 4-day survival. For the F1 generation 4-day survival, 449 mg/kg bw/day was estimated as BMDL5. The corresponding MLE dosages were 786 (polynomial model) and 771 mg/kg bw/day (Weibell model) for the reproductive effects, 656 mg/kg bw/day for the F1 postnatal effects, and 804 mg/kg bw/day for the F2 postnatal effects.

Shipp, A.M., Allen, B.C., Van Landingham, C., Gentry, P.R. and Crump, K.S., Quantitative Dose-Response Analysis -- Application of the Benchmark Method to the Multi-Generation Rat Reproduction Study for Isopropanol. Final Report prepared by ICF Kaiser, KS

	Crump Division, 602, East Georgia Avenue, Ruston, Louisiana for Chemical Manufactureres Association Isopropanol Panel, Apri11996.
Type	One generation study
Species	rat
Strain	Wistar
Sex	male/female
Route of Administration	drinking water
Exposure Period	prior to mating and to lactation and weaning of Fl generation
Frequency of Treatment	continuous
Premating Exposure Period	
male	8 weeks
female	8 weeks
Duration of Test	
Doses	2 and 3% isopropanol in drinking water
Control Group	yes
NOEL Parental	=2%
NOEL FI Offspring	=2%
NOEL F2 Offspring	
Method	other
Year	1977
GLP	no
Test Substance	> 99.7% (w/w) 2-propanol
Remark	Isopropanol was administered as a 3% solution in the drinking water. Reduced parental body weight gain, food and water consumption were observed in the isopropanol-treated animals compared with controls. In addition, fertility, litter size, and pup weights at postnatal days 4 and 21 were reduced in the 3% treatment group compared with the controls. The dose was dropped to 2% isopropanol and the parental animals were re- mated to provide litters for a developmental toxicity evaluation. No parental toxicity or reproductive toxicity was noted.
Reference	Gallo, M.A., Oser, B.L, Cox, G.E., and Bailey, D.E. (1977) Toxicol. Appl. Pharmacol. 41:35

5.8.2 Developmental Toxicity/Teratogenicity

Species	rat
Strain	Wistar
Sex	female
Route of Administration	drinking water
Exposure Period	Days 6 - 16 of pregnancy.
Frequency of Treatment	continuous
Duration of Test	To day 20 of pregnancy.
Doses	0.5, 1.25, 2.5%

Control Group	yes
NOEL Maternal	=0.5%
Toxicity NOEL	=0.5%
Teratogenicity Method	other
Year	1986
GLP	yes
Test Substance	> 99.7% (w/w) 2-propanol
Remark	Maternal body weights were significantly decreased from gestational days 7-16. Animals in the 1.25% and 2.5% dose groups exhibited reduced food and water consumption during the treatment period. In the 1.25% and 2.5% dose groups, fetal body weights were reduced on a per fetus basis, but not on a per litter basis. No teratogenic effects were observed; but, delayed ossification of the skeleton was noted in the 1.25% and 2.5% dose groups, consistent with rewded development as a result of matemal toxicity.
Reference	British Industrial Biological Research Assoc., Report no. 0570/2/86.

Species	rat
Strain	Sprague- Dawley
Sex	female
Route of Administration	gavage
Exposure Period	6 - 15 of gestation
Frequency of Treatment	daily
Duration of Test	To day 20 of pregnancy
Doses	0, 400, 800 and 1200 mg/kg/day
Control Group	yes
NOEL Maternal	= 400 mg/kg bw/day
Toxicity NOEL	
Developmental	= 400 mg/kg bw/day
Toxicity	other (US EPA TCSA Test Guidelines) 1994
Method	1994
Year	yes
GLP	> 99.7% (w/w) 2-propanol
Test Substance	No dams aborted or delivered early. Two dams died at 1200 mg/kg
Remark	and one dam died at 800 mg/kg. Reduced maternal gestational weight gain on gestational days 0 to 20 associated with significantly reduced gravid uterine weights were noted in the high-dose animals. All gestational parameters were equivalent across groups. Fetal body weights per liter were significantly reduced at the two highest doses. There were no adverse maternal or developmental effects at 400 mg/kg. No evidence of increased teratogenicity was observed at any dose tested. Therefore, isopropanol was not teratogenic to CD rats.
Reference	Tyl, RW., Masten, L.W., Marr, M.C., Myers, C.B., Slauter, R.W., Gardiner, T.R, Strother, D.E., McKee, RH., and Tyler, T.R (1994) Fundam. Appl. Toxicol. 22:139- 151.

Species	rabbit
Strain	New Zealand white
Sex	female
Route of Administration	gavage
Exposure Period	Days 6 - 18 of pregnancy
Frequency of Treatment	daily
Duration of Test	to day 28 of pregnancy 1
Doses	20, 240 and 480 mg/kg/day
Control Group	yes
NOEL Maternal	= 240 mg/kg bw/day
Toxicity NOEL	
Developmental	= 480 mg/kg bw/day
Toxicity	other (US EPA TCSA Test Guidelines)
Method	1994
Year	yes
GLP	> 99.7% (w/w) 2-propanol
Test Substance	No does aborted or delivered early. Four does died at 480 mg/kg.
Remark	Maternal body weights were significantly reduced during treatment and clinical signs of toxicity were observed at 480 mg/kg. No adverse maternal effects were noted at 120 or 240 mg/kg. All gestational parameters were equivalent across groups. No evidence of increased teratogenicity was observed at any dose tested. Therefore, isopropanol was not teratogenic to NZW rabbits.
Reference	Tyl, RW., Masten, L.W., Marr, M.C., Myers, C.B., Slauter, RW., Gardiner, T.H., Strother, D.E., McKee, R.H., and Tyler, T.R (1994) Fundam. Appl. Toxicol. 22: 139- 151.

Species	rat
Strain	Sprague- Dawley
Sex	female
Route of Administration	gavage
Exposure Period	day 6 of pregnancy to day 21 postnatal.
Frequency of Treatment	daily
Duration of Test	Day 68 post natal.
Doses	200, 700 and 1200 mg/kg/day
Control Group	yes
NOEL Maternal Toxicity	= 700 mg/kg bw/day
NOEL Developmental	
Neurotoxicity	= 1200 mg/kg bw/day
Method	other (US EPA TCSA Test Guidelines)
Year	1994
GLP	yes
Test Substance	> 99.7% (w/w) 2-propanol
Remark	This study was specifically designed to investigate developmental neurotoxicity. One high-dose dam died on postnatal day 15, but there were no other clinical observations or effects on maternal

	weight, food consumption, or gestation length. Pup survival, weight, sex ratio, and sexual maturation were unaffected. There were no biologically significant findings in the behavioral tests, no changes in organ weights, and no pathological findings that could be attributed to isopropanol exposure.
Reference	Bates, H.K., McKee, R.H., Bieler, G.S., Gardiner, T.H., Gill, M.W., Strother, D.E., and Masten, L.W. (1994) Fundam. Appl. Toxicol. 22:152-158.

Species	rat
Strain	Sprague- Dawley
Sex	
Route of Administration	inhalation
Exposure Period	gestational days 1-19
Frequency of Treatment	7 hours/day
Duration of Test	gestational day 20
Doses	3500,7000 and 10000 ppm
Control Group	yes
NOEL Maternal	= 3500 ppm
Toxicity NOEL	< 3500 ppm
Teratogenicity Method	not specified
Year	1988
GLP	yes
Test Substance	
Remark	The animals showed unsteady gait and narcotization during initial exposures in the mid- and high-dose groups; reduced food consumption and reduced weight gain were also noted in both the mid- and high-dose groups. Fetal body weights per litter were reduced in all dose groups. Exposure to 10000 ppm also resulted in failure of implantation, fully resorbed litters, increased resportions per litter and increased incidence of cervical ribs.
Reference	Nelson, B.K., Brightwell, W.S., MacKenzie-Taylor, DR, Khan, A., Burg, J.R., and Weigel, W.W. (1988) Fd. Chem. Toxicol. 26: 247254.

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2 Physico-chemical Properties

2.1 Melting Point

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Value	= -114°C
Sublimation	
Method	
Year	1953
GLP	no data
Test substance	other TS: USI absolute
Method	Freezing and melting points determined in a stirred cell designed to protect contents from contact with atmosphere. The cell was surrounded with a clear glass dewar flask which provided uniform changes in temperature when the assembly was immersed in cooling or warming baths. The temperature in the cell was measured with a copper-constantan thermocouple inserted into a thermcouple well which contained n-propyl alcohol as a thermal conducting medium. The thermocouple was calibrated by measuring the freezing points of purified materials. Freezing points of benzene, water, carbon tetrachloride, mercury, chloroform and toluene were determined and a correction curve plotted. From this curve a correction was applied to the freezing points of the mixtures being studied. Cooling was using liquid nitrogen.
Remark	The authors noted that ethanol was prone to supercooling.
Reliability	(2) valid with restrictions Critical study for SIDS endpoint
Reference	Corcoran, J., Kruse, H. and Skolnik, S. (1953). Thermal analysis of the systems hydrazinemethanol and hydrazine-ethanol. J. Phys. Chem. 57: 435-437.
11.09.2002	(25)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Value	=-114.1 degree C
Decomposition	no
Sublimation	no
Method	other
Year	
GLP	
Test substance	95 – 99.9% ethanol (64-17-5)
Method	
Remark	Method not specified. Value after Corcoran, J., Kruse, H. and Skolnik, S. (1953) Thermal analysis of the systems hydrazine-methanol and hydrazine-ethanol. J. Phys.

Chem. 57: 435-437.
Reliability (2) valid with restrictions
Reference Merck (1996) The Merck Index 12th edition, Merck & Co., Inc., Rahway, New Jersey.
16.01.2004 (26)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Value: -89.90 degree C
Method: Method not listed.
GLP: No
Test substance: 99.9% 1-butanol (71-36-3)
Reliability: (2) Valid with restrictions, full experimental details are not available.

Reference: Union Carbide Corporation, Solvents & Coatings Materials Division. Material Safety Data Sheet: C0296F, Dated 10/18/95

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = -44 - -51 degree C

Test substance: >95% 1-hexanol (111-27-3)

Reliability: (4) not assignable
Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.
Flag: Critical study for SIDS endpoint
31-DEC-2004 (77)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = -51.6 degree C

Method: other: not specified
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. (Reference: Registry of Toxic Effects of Chemical Substances)

Reference: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
03-JAN-2005

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = -15.5 to -17 degree C

Test substance: > 90% 1-octanol (111-87-5)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
Flag: Critical study for SIDS endpoint
Reference: Budavari, S. (ed.). 1996. Merck Index. 12th ed. Whitehouse Station: Merck Research Laboratories.
03-JAN-2005 (31)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = -18 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Safety data sheet Henkel KGaA
03-JAN-2005 (95)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = -16.7 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Sax, I. & Lewis, R.J (eds.). "Dangerous Properties of Industrial Materials", 2nd edition, Vol. III, Van Nostrand

Reinhold, New York (1989)
03-JAN-2005 (97)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = -16.7 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Sax, I. & Lewis, R.J (eds.). "Dangerous Properties of Industrial Materials", 2nd edition, Vol. III, Van Nostrand Reinhold, New York (1989)
03-JAN-2005 (97)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = -16.3 degree C

Test substance: > 90% 1-octanol (111-87-5)

Reliability: (4) not assignable
Documentation insufficient for assessment
Reference: Lington, A.W. and Bevan, C.1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
03-JAN-2005 (78)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 6.4 degree C

Test substance: > 90% 1-decanol (112-30-1)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
Flag: Critical study for SIDS endpoint
References: Budavari, S. (ed.). 1996. Merck Index. 12th ed. Whitehouse Station: Merck Research Laboratories.

Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

03-JAN-2005 (20) (63)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = -7 degree C

Test substance: > 90% 1-decanol (112-30-1)

Reliability: (4) not assignable

Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.

03-JAN-2005 (100)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 6.9 degree C

Test substance: > 90% 1-decanol (112-30-1)

Reliability: (4) not assignable
Value obtained from secondary literature. Original reference not stated.

Reference: Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.

03-JAN-2005 (87)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 3 to 6 degree C

Decomposition: no at degree C

Sublimation: no

Test substance: > 90% 1-decanol (112-30-1)

Source: Henkel KGaA Duesseldorf

Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.

Reference: Safety data sheet, Henkel KgaA

03-JAN-2005 (75)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 4 to 7 degree C
Decomposition: no
Sublimation: no

Test substance: > 90% 1-decanol (112-30-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.

Reference: Safety data sheet, Henkel KgaA
03-JAN-2005 (75)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 7 degree C

Test substance: > 90% 1-decanol (112-30-1)

Source: Henkel KGaA Duesseldorf
Reliability: (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference cited is an authoritative, peer-reviewed
secondary data source
Reference: Beilstein ONLINE.
03-JAN-2005 (14)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Value: = 22.6 to 24 degree C

Test substance: Dodecanol (112-53-8)

Source: Budavari 1996.
Reliability: (4) not assignable
Reference: Budavari, S. (ed.). 1996. Merck Index. 12th ed.
Whitehouse Station: Merck Research Laboratories.
24-SEP-2003 (2)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 39.5 degree C
Test substance: 1-Tetradecanol
Source: Henkel KGaA Duesseldorf
Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. Original reference not stated.
Flag: Critical study for SIDS endpoint
Reference: Weast, R.C., CRC Handbook of chemistry and physics, CRC Press, Cleveland, Ohio, C-512 (1977/78).
21-OCT-2005 (81)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 39.5 degree C

Test substance: > 95% 1-Tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
Assessment performed according to accepted models and principles.
Reference: Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.
21-OCT-2005 (71)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 38 degree C

Test substance: > 95% 1-Tetradecanol (112-72-1)

Reliability: (4) not assignable
Documentation insufficient for assessment.
Reference: Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
21-OCT-2005 (47)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 35 to 38 degree C

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Safety data sheet Henkel KgaA
21-OCT-2005 (59)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 37.4 - 37.7 degree C

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint
Reference: Safety data sheet Henkel KgaA
21-OCT-2005 (59)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 37.8 degree C

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Egan, R.R. & Portwood, O., Cosmet. Perfum. 89, 39-42 (1974)
21-OCT-2005 (16)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 38 degree C

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf

Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Henkel, Fettchem. Tabellen, 3. Aufl., Duesseldorf (1971)
21-OCT-2005 (38)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 50 degree C

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The cited source of the value is a recognised source of physico-chemical data.
Flag: Critical study for SIDS endpoint
Reference: Weast, R.C., CRC Handbook of chemistry and physics, 58th ed., CRC Press, Cleveland, C-332 (1977/78).
04-JAN-2005 (99)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: ca. 46 to 52 degree C
Decomposition: no
Sublimation: no

Method: other
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source: UNION DERIVAN S.A. VILADECANS
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified. A source of higher reliability is available.
Reference: UNION DERIVAN S.A. VILADECANS
19-SEP-2005

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 49 degree C

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Noweck, K. & Ridder, H., Ullmann's encyclopedia of industrial chemistry, 5th ed., Vol. A10, VCH, Weinheim, 277-296 (1987).
19-SEP-2005 (64)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 49.3 degree C

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Henkel, Fettchem. Tabellen, 3. Aufl., Duesseldorf, 24-25 (1971)
19-SEP-2005 (44)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Value: = 59.5 degree C

Test substance: Octadecanol (112-92-5)

Source: SRC.
Reliability: (4) not assignable
Reference: Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.
24-SEP-2003 (14)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Value: = 58 degree C

Test substance: octadecanol (112-92-5)

Source: Lington and Bevan 1994.
Reliability: (4) not assignable
Reference: Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
24-SEP-2003 (10)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Value: = 66 degree C

Test substance: octadecanol (112-92-5)

Reliability: (4) not assignable
Documentation insufficient for assessment.
Flag: Critical study for SIDS endpoint
Reference: Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
04-JAN-2005 (14)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Value: = 64 - 68 degree C

Method: other: DAB 10 V.6.11.1
GLP: no
Test substance: >= 90% 1-eicosanol (629-96-9)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Technical data sheet for NACOL 20-96, Condea Chemie GmbH, 1993.
04-JAN-2005 (21)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Value: = 72.5 degree C

Test substance: >95% 1-docosanol (661-19-8)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data.
Flag: Critical study for SIDS endpoint
Reference: Lide, D.R. (ed.). 1999. CRC Handbook of Chemistry and Physics. 80th ed. Boca Raton: CRC Press.
04-JAN-2005 (20)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Value: = 69 - 73 degree C

Method: other: DAB 10 V.6.11.1
GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: NACOL 22-98 Material Safety Data Sheet. RWE-DEA AG fur Mineraloel und Chemie. Version 2.00.00 Int. no. 2298502, 1994.
04-JAN-2005 (25)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Value: = 71 degree C

GLP: no data
Test substance: >95% 1-docosanol (661-19-8)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Chemical Rubber Company Atlas of Spectral Data and Physical Constants for Organic Compounds. CRC Press, Cleveland,Ohio, second edition, 1975.
04-JAN-2005 (8)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Value: = 74 to 76 degree C

Method: unknown
GLP: unknown
Test substance: 1-tetracosanol (506-51-4)

Reliability: (4) not assignable
Reference: Al Dulayymi, Juma'a R.; Tetrahedron 2005 V61(50) pp. 11939-51. Available at STN.

04-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Value: = 77 to 78 degree C

Method: unknown
GLP: unknown
Test substance: 1-hexacosanol (506-52-5)

Reliability: (4) not assignable
Reference: Li, Jiren; Zhongguo Zhongyao Zazhi 2002 V27(1) pp. 40-42. Availabel at STN.
04-APR-2007

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Value: = 80 to 82 degree C

Method: uknown
GLP: unknown
Test substance: 1-octacosanol (557-61-9)

Reliability: (4) not assignable
Reference: Saraswathy, A.; Indian Drugs 1990 V27 (7) pp. 399-400. Available at STN.
04-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Value: = 87 degree C

Method: unknown
GLP: unknown
Test substance: 1-triacontanol (593-50-0)

Reliability: (4) not assignable
Reference: Merck (1996). The Merck Index. 12th Edition. Merck and Company, Inc., Whitehouse Station, New Jersey. From BIBRA Information Services Ltd. (1997) Toxicity Profile: Triacontanol. Sutton, Surrey.
04-APR-2007

2.2 Boiling Point

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Value	= 78.3 degree C at 1013.25 hPa
Decomposition	no
Method	other
Year	1970
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Comparative ebulliometry. The apparatus used is described in detail in one of the references along with a detailed description of its operation. The two boilers (reference plus test substance) are connected by a common pressure line. Platinum resistance thermometers are used to measure the temperature using a Mueller bridge. Water was used as the reference substance. The method is reported to be repeatable to within a few thousandths of a degree.
Result	The results consist of two sets of readings for the thermometers, one for the sample and one for the standard. The data was processed by computer to establish the best fit Antoine and Kirchoff equations. The source of the reference data for water is quoted and any necessary corrections are described. The result is quoted as 351.443K and is corrected for the freezing point of water of 273.15K.
Source	Riddick JA, Bunger WB, Sakano TK (1986), Techniques of Chemistry, Vol 1l, Organic Solvents, Physical Properties and Methods of Purification, Wiley
Test Substance	Samples purified before use, including drying in vapour phase. Fraction molarity purity 0.9995.
Reliability	(2) valid with restrictions Whilst old and not to an OECD protocol, the method and technique is well reported.
Flag	Critical study for SIDS endpoint
References	Ambrose D (1968), Improved boilers for the ebulliometric determination of vapour pressures, J Sci Instrum (J Physics E), series 2, vol 1, p 41. Ambrose D, Sprake CHS (1970), Thermodynamic properties of organic oxygen compounds. XXV. Vapour pressures and normal boiling temperatures of aliphatic alcohols.

	J Chem Thermodynam, 2, 631-45
09.11.2004	(27) (28)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Value	78 degree C at 760 hPa
Decomposition	No
Method	other
Year	1951
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Source	Budavari, S., (ed.) (1996). The Merck Index. 12th Ed. Merck&Co: Whitehouse Station, NJ.
Reliability	(2) valid with restrictions
Reference	McKenna, F., Tartar, H., Lingfeiter, S. (1953). Studies of hemiacetal formation in alcohol-aldehyde systems: refraction studies. J. Amer. Chem. Soc. 75.604-607.
09.11.2004	(29)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Value	= 78.5 degree C
Decomposition	
Method	other: IP71 section 1/97 1997
Year	
GLP	
Test substance	other TS: double rectified absolute alcohol
Source	Data generated by SG Redwood (UK) Ltd, IS09002 No Q4856
Reliability	(2) valid with restrictions
Reference	BP Chemicals Ltd. Internal data 1997, 1998 and 1999.
09.11.2004	(30)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Value	= 78.2 degree C
Decomposition	no
Method	other
Year	
GLP	no data
Test substance	no data
Remark	Method not specified.
Reliability	(4) not assignable
Reference	Merck (1989) The Merck Index 11th edition, Merck & Co., Inc., Rahway, New Jersey.

29.09.2003 (31)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Value: 117.60 degree C at 101.325 kP.
Method: Method not listed.
GLP: No

Reliability: (2) Valid with restrictions, full experimental details are not available.

Reference: Union Carbide Corporation, Solvents & Coatings Materials Division Material Safety Data Sheet: C0296F, Dated 10/18/95.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 158 degree C

Test substance: >95% 1-hexanol (111-27-3)

Reliability: (4) not assignable
Flag: Critical study for SIDS endpoint
Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.
03-JAN-2005 (77)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 145 - 160 degree C

Method: other: DIN 51751
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Source: Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: MSDS Henkel KGaA. Lorol C 6 (DED 00003640 00, Ausgabe 01 vom 21.04.1994).
03-JAN-2005 (40)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 150 to 170 degree C

Method: other: ASTM-D-1078
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Material Safety Data Sheets, NACOL 6-97 and NACOL 6M, Condea Chemie GmbH, Version 1.00.02, Int. no. 699003, 1994)
03-JAN-2005 (35)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 152 to 162 degree C

Method: other: ASTM-D-1078
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: NACOL 6-99 Material Safety Data Sheet. RWE-DEA AG für Mineraloel und Chemie. Version 1.00.02, int. no. 699003, 1994.
03-JAN-2005 (42)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 157 degree C

Method: other: not specified
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000

CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.

Reference: Registry of Toxic Effects of Chemical Substances, online search 1995.

03-JAN-2005 (51)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 194 to 195 degree C

Test substance: > 90% 1-octanol (111-87-5)

Reliability: (2) valid with restrictions

Value obtained from a recognised source of physico-chemical data

Flag: Critical study for SIDS endpoint

Reference: Budavari, S. (ed.). 1996. Merck Index. 12th ed. Whitehouse Station: Merck Research Laboratories.

03-JAN-2005 (31)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 185 to 210 degree C at 1013 hPa

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf

Reliability: (4) not assignable

This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.

Reference: Safety data sheet Henkel KGaA

03-JAN-2005 (95)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 194.5 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf

Reliability: (4) not assignable

This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.

Reference: Sax, I. & Lewis, R.J (eds.). "Dangerous Properties of

Industrial Materials", 2nd edition, Vol. III, Van Nostrand Reinhold, New York (1989)

03-JAN-2005 (97)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 229 degree C at 1013 hPa

Test substance: > 90% 1-decanol (112-30-1)

Source: Henkel KGaA Duesseldorf

Reliability: (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference cited is an authoritative, peer-reviewed
secondary data source

Flag: Critical study for SIDS endpoint

Reference: Beilstein ONLINE.

11-OCT-2005 (14)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 231 - 234 degree C

Test substance: > 90% 1-decanol (112-30-1)

Reliability: (4) not assignable
Documentation insufficient for assessment.

References: Gerarde, H.W. and Ahlstrom, D.B. 1966. Aspiration hazard and toxicity of a homologous series of alcohols. Arch. Environ. Health 13:457-461.

Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

03-JAN-2005 (28) (63)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 220 to 235 degree C at 1013 hPa

Test substance: > 90% 1-octanol (111-87-5)

Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the

reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.

Reference: Safety data sheet, Henkel KgaA

03-JAN-2005 (75)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 220 to 240 degree C at 1013 hPa

Test substance: > 90% 1-decanol (112-30-1)

Source: Henkel KGaA Duesseldorf

Reliability: (4) not assignable

This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.

Reference: Safety data sheet, Henkel KgaA

03-JAN-2005 (75)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Value: = 255 to 269 degree C

Test substance: Dodecanol (112-53-8)

Source: Verschueren 1996.

Reliability: (4) not assignable

Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.

24-SEP-2003 (25)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Value: = 259 degree C at 1013 hPa

Test substance: dodecanol (112-53-8)

Source: Budavari 1996.

Reliability: (4) not assignable

Reference: Budavari, S. (ed.). 1996. Merck Index. 12th ed. Whitehouse Station: Merck Research Laboratories.

24-SEP-2003 (2)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 289 degree C

Test substance: > 95% 1-tetradecanol (112-72-1)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
Flag: Critical study for SIDS endpoint
Reference: Lide, D.R. (ed.). 1999. CRC Handbook of Chemistry and Physics. 80th ed. Boca Raton: CRC Press.
04-JAN-2005 (46)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 263.2 degree C at 1013 hPa

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Weast, R.C., CRC Handbook of chemistry and physics, CRC Press, Cleveland, Ohio, C-512 (1977/78)
04-JAN-2005 (81)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 264 degree C at 1013 hPa

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Neumueller, O.-A., Roempps Chemie-Lexikon, S. Aufl., Franckh""sche Verlagshandlung, Stuttgart, 4182, (1988).
04-JAN-2005 (52)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 280 to 300 degree C at 1013 hPa

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Safety data sheet Henkel KgaA
04-JAN-2005 (59)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 285 to 300 degree C at 1013 hPa

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Safety data sheet Henkel KgaA
04-JAN-2005 (59)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 296.2 degree C at 1013 hPa

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Boublik,T. et al., "The Vapour Pressures of Pure Substances", Elsevier Scientific Publishing Company, Amsterdam (1973).
04-JAN-2005 (9)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 334 to 344 degree C

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data.
Flag: Critical study for SIDS endpoint
Reference: Lide, D.R. (ed.). 1999. CRC Handbook of Chemistry and Physics. 80th ed. Boca Raton: CRC Press.
17-OCT-2005 (54)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 300 to 320 degree C

Method: other
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source:
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified. A source of higher reliability is available.
Reference: UNION DERIVAN S.A. VILADECANS
04-JAN-2005

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 344 degree C at 1013 hPa

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Weast, R.C., CRC Handbook of chemistry and physics, 58th ed., CRC Press, Cleveland, C-332 (1977/78)
04-JAN-2005 (99)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Value: = 210 degree C

Test substance: octadecanol (112-92-5)

Remark: Test conducted at a pressure of 15 mmHg
Source: Budavari 1996.
Reliability: (4) not assignable
Reference: Budavari, S. (ed.). 1996. Merck Index. 12th ed. Whitehouse Station: Merck Research Laboratories.
24-SEP-2003 (1)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Value: = 309 degree C

Test substance: : >= 90% 1-eicosanol (629-96-9)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
Flag: Critical study for SIDS endpoint
Reference: Lide, D.R. (ed.). 1999. CRC Handbook of Chemistry and Physics. 80th ed. Boca Raton: CRC Press.
04-JAN-2005 (13)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Value: = 372 degree C

Test substance: : >= 90% 1-eicosanol (629-96-9)

Reliability: (4) not assignable
Value obtained from secondary literature. Original reference not stated.
Reference: Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.
04-JAN-2005 (20)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Value: = 401.1 degree C

Method: other: calculated (SRC MPBPVP v1.40)
Year: 2004
GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Remark: The presence of branched components in the substance is expected to raise the boiling point of those substances slightly, though it is not possible to predict values precisely. Validation of boiling point prediction using this method shows that the calculated values are very close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the values estimated by MPBPVP.
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
11-OCT-2005 (1)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Value: = 180 degree C

Test substance: >95% 1-docosanol (661-19-8)

Remark: Test conducted at a pressure of 0.22 mm Hg.
Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
Reference: Lide, D.R. (ed.). 1999. CRC Handbook of Chemistry and Physics. 80th ed. Boca Raton: CRC Press.
11-OCT-2005 (20)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Value: = 180 degree C

GLP: no data
Test substance: >95% 1-docosanol (661-19-8)

Remark: by comparison with other measured values, it is considered likely that this result was obtained at reduced pressure.
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Chemical Rubber Company Atlas of Spectral Data and Physical Constants for Organic Compounds. CRC Press, Cleveland,Ohio,

second edition, 1975
11-OCT-2005 (8)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Value: = 230 to 235 degree C at 12 Torr

Method: unknown
GLP: unknonw
Test substance: 1-Tetracosanol (506-51-4)
Reliability: (4) not assignable
Reference: Sulzbacher, Max; GB 712043 1954. Available at STN.
04-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Value: = 175 degree C at 0.02 Torr

Method: unknown
GLP: unknown
Test substance: 1-hexacosanol (506-52-5)
Reliability: (4) not assignable
Reference: Jacini, Giovanni; Gazzeta Chimica Italiana 1947 V77, pp. 247-51. Available at STN.
04-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Value: = 305 degree C at 20 Torr

Method: unknown
GLP: unknown
Test substance: 1-hexacosanol (506-52-5)
Reliability: (4) not assignable
Reference: CRC Press (1997). CRC Handbook of Chemistry and Physics. 75th Edition. CRC Press, Boca Raton.
04-APR-2007

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Value: = 470.70 degree C

Method: other: calculated (SRC MPBPVP v1.41)
Year: 2007
GLP: no
Test substance: 1-octacosanol (557-61-9)

Remark: The presence of branched components in the substance, within is expected to raise the boiling point of those substances slightly, though it is not possible to predict values precisely. Validation of boiling point prediction using this method shows that the calculated values are very close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: SRC MPBPVP v1.41. U.S. EPA, 2006.
04-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Value: = 493.91 degree C

Method: other: calculated (SRC MPBPVP v1.41)
Year: 2007
GLP: no
Test substance: 1-triacontanol (593-50-0)

Remark: The presence of branched components in the substance, within is expected to raise the boiling point of those substances slightly, though it is not possible to predict values precisely. Validation of boiling point prediction using this method shows that the calculated values are very close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: SRC MPBPVP v1.41. U.S. EPA, 2006.
04-APR-2007

2.3 Density

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Density
Value	= 0.7864 g/cm^3 at 25°C
Method	other
Year	1984
GLP	no data

Test substance	95 – 99.9% ethanol (64-17-5)
Method	Density determined using an oscillating tube densitometer DMA 60/61 (from Paar). The density is determined by measuring the natural vibration frequency of a U shaped glass tube filled with the test fluid. The density is related to the period of oscillation of the instrument but can be calculated relative to a known substance, in this case water, by the equation: Ds - Dw = Ax (Ts2 - Tw2) where Ds and Dw are densities of substance and water, and Ts2 and Tw2 are the oscillation periods to the power of 2 of the test substance and water respectively. The constant A can be determined by making measurements with water and air. (Density values for water from reference Kell (1975) The temperature was maintained within 0.002K and measured using a calibrated quartz thermometer. Water content was checked using a Karl Fisher titration apparatus.
Result	Results available at 5, 15, 25, 35 and 45 degree C to an accuracy of 0.01 degree C and 2E6 for density.
Source	Riddick JA, Bunger WB, Sakano TK (1986), Techniques of Chemistry, Vol II, Organic Solvents, Physical Properties and Methods of Purification, Wiley
Test substance	Ethanol dried over a molecular sieve 3A then fractionally distilled. Water reference deionised then distilled using a quartz still.
Reliability	(2) valid with restrictions Not to a standard OECD protocol but reported in detail and considered reliable
Flag	Critical study for SIDS endpoint
References	Sakurai M, Nakagawa T (1982) Densities of dilute solutions of benzene and methanol at 278.15, 288.15, 298.15, 308.15 and 318.15K. Partial molar volumes Vw and values of dVw/dT for water in benzene and methanol. J Chem Thermodynam, 14, 269-74 Sakurai M, Nakagawa T (1984), Densities of dilute solutions of water in n-alkanols at 278.15, 288.15, 298.15, 308.15 and 318.15K. Partial molar volumes of water in n-alkanols. J Chem Thermodyn, 16, 171.
11.11.2004	(32) (33)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	relative density
Value	= .7896 at 20°C
Method	other: IP365/97 1997
Year	
GLP	
Test substance	other TS: double rectified absolute alcohol

Remark	Test performed by SG Redwood (UK) Ltd. IS09002. no Q4856
Reliability	(2) valid with restrictions
Reference	BP Chemicals Ltd. Internal data 1997, 1998 and 1999.
11.11.2004	(30)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	relative density
Value	= .789 at 20 degree C
Method	other
Year	
GLP	
Test substance	95 – 99.9% ethanol (64-17-5)

Remark	
Reliability	(4) not assignable
Reference	Merck (1989) The Merck Index 11th edition, Merck & Co., Inc., Rahway, New Jersey.
29.09.2003	(31)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Density
Value	= .7892 - .7896 at 20 degree C
Method	other: ASTM D4052 2003
Year	
GLP	
Test substance	

Remark	Sales specification for ethanol.
Test Substance	>99.9% ethanol
Reliability	(2) valid with restrictions Routine property measured to standard method.
Reference	BP Chemicals Ltd, Sales specification (2003)
18.10.2004	(34)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Value:	0.8097
Comments:	Calculated at 20/4°C
Test substance:	99.9% 1-butanol (71-36-3)
Reliability:	(2) Valid with restrictions, full experimental details are not available.
Reference:	Othmer, Kirk. 3rd Edition 21:378. Beilstein a. E III. 2: b. E IV 113.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Value: 0.8098 g/cm^3 @ 20° C
Test substance: 99.9% 1-butanol (71-36-3)
Reliability: (2) Valid with restrictions, full experimental details are not available.

Reference: (Weast and Astle, 1985)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = .82

Test substance: >95% 1-hexanol (111-27-3)

Source: Chemfinder
Reliability: (4) not assignable
This value was obtained from secondary literature.
Flag: Critical study for SIDS endpoint
Reference: http://chemfinder.cambridgesoft.com/
03-JAN-2005 (27)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: density
Value: = .81 - .82 g/cm³ at 20 degree C

Method: other: DIN 51757 B
Test substance: >95% 1-hexanol (111-27-3)

Source: Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: MSDS Henkel KGaA. Lorol C 6 (DED 00003640 00, Ausgabe 01 vom 21.04.1994)
03-JAN-2005 (40)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: density
Value: = 817 - 821 g/cm³ at 20 degree C

Method: other: DIN 51757
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Material Safety Data Sheets, NACOL 6-97 and NACOL 6M, Condea Chemie GmbH, Version 1.00.02, Int. no. 699003, 1994)
03-JAN-2005 (35)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = .826

Test substance: > 90% 1-octanol (111-87-5)

Reliability: (4) not assignable
Value obtained from secondary literature.
Flag: Critical study for SIDS endpoint
Reference: Value obtained from the Chemfinder website at http://chemfinder.cambridgesoft.com/
21-OCT-2005 (118)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = .82 - .83

Test substance: > 90% 1-octanol (111-87-5)

Remark: Test conducted at 20 degrees C
Reliability: (4) not assignable
Reference: IUCLID data sheet. 1995j. Octanol.
11-OCT-2005 (63)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: density
Value: = .815 - .825 g/cm³ at 20 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf

Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Safety data sheet Henkel KGaA
03-JAN-2005 (95)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: density
Value: = .8254 at 20 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Fettchemische Tabellen, 3. Aufl., Henkel KGaA (1971).
03-JAN-2005 (40)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: density
Value: = .827 at 20 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Sax, I. & Lewis, R.J (eds.). "Dangerous Properties of Industrial Materials", 2nd edition, Vol. III, Van Nostrand Reinhold, New York (1989)
03-JAN-2005 (97)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: density
Value: = .8297 g/cm³ at 20 degree C

Test substance: > 90% 1-decanol (112-30-1)

Source: Henkel KGaA Duesseldorf
Reliability: (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference cited is an authoritative, peer-reviewed
secondary data source
Flag: Critical study for SIDS endpoint
Reference: Beilstein ONLINE.
03-JAN-2005 (14)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = .83

Test substance: > 90% 1-decanol (112-30-1)

Reliability: (4) not assignable
Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.
03-JAN-2005 (100)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: density

Value: = .82 - .83 g/cm³ at 20 degree C

Test substance: > 90% 1-decanol (112-30-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Safety data sheet, Henkel KgaA
03-JAN-2005 (75)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Value: = .83

Test substance: dodecanol (112-53-8)

Source: SIDS Dossier on 1-Dodecanol 1993a.
Reliability: (2) valid with restrictions
Reference: SIDS Dossier on 1-Dodecanol. 1993a. Environmental Protection Agency, Denmark. 6 June 1993.
01-OCT-2003 (19)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Type: density
Value: = .8236 g/cm³ at 38 degree C

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Flag: Critical study for SIDS endpoint
Reference: Henkel, Fettchem. Tabellen, 3. Aufl., Duesseldorf (1971)
11-OCT-2005 (38)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Type: density
Value: = .8355 g/cm³ at 20 degree C

Test substance: > 95% 1-Tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Sax, N.I. & Lewis, R.J., Hawley's condensed chemical dictionary, 11th ed, Van Nostrand Reinhold Co., New York (1987).
11-OCT-2005 (61)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Type: density

Value: = .81 - .82 g/cm³ at 40 degree C

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Safety data sheet Henkel KgaA
11-OCT-2005 (59)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = .823 g/cm³

Test substance: > 95% 1-tetradecanol (112-72-1)

Reliability: (4) not assignable
Value obtained from secondary literature. Original reference not stated.
Reference: Value obtained from the Chemfinder website at http://chemfinder.cambridgesoft.com/
21-OCT-2005 (77)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: density
Value: = .8176 g/cm³ at 50 degree C

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Flag: Critical study for SIDS endpoint
Reference: Henkel, Fettchem. Tabellen, 3. Aufl., Duesseldorf, 24-25 (1971)
17-OCT-2005 (44)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = .818

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Reliability: (4) not assignable
Value obtained from secondary literature. Original reference not stated.
Reference: Value obtained from the Chemfinder website at http://chemfinder.cambridgesoft.com/
21-OCT-2005 (92)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: density
Value: ca. .81 g/cm³ at 60 degree C

Method: other
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.
Reference: UNION DERIVAN S.A. VILADECANS
04-JAN-2005

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Value: = .812 at 59 degree C

Test substance: Octadecanol (112-92-5)

Source: SIDS Dossier on 1-Octadecanol 1993b.
Reliability: (4) not assignable
Reference: SIDS Dossier on 1-Octadecanol. 1993b. Environmental Protection Agency, Denmark. 6 June 1993.
30-SEP-2003 (12)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Type: relative density
Value: = .8405 at 20 degree C

Test substance: **:** >= 90% 1-eicosanol (629-96-9)

Source: HSDB
Reliability: (2) valid with restrictions

Value obtained from secondary literature (HSDB). Cited reference is a recognised source of chemical data
Flag: Critical study for SIDS endpoint
Reference: Weast, R.C. (ed.). Handbook of Chemistry and Physics. 60th ed. Boca Raton: CRC Press Inc., 1979.C-283.
04-JAN-2005 (25)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Type: density
Value: = .8 - .804 g/cm³ at 4 degree C

Method: other: DIN 51757
GLP: no
Test substance: >= 90% 1-eicosanol (629-96-9)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Material Safety Data Sheets, NACOL 20-95 and NACOL 20-96, Condea Chemie GmbH, 1994.
04-JAN-2005 (15)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Type: density
Value: = .805 - .809 g/cm³ at 4 degree C

Method: other: DIN 51757
GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Review of the original source (secondary literature) would not alter the reliability of this result.
Flag: Critical study for SIDS endpoint
Reference: NACOL 22-98 Material Safety Data Sheet. RWE-DEA AG fur Mineraloel und Chemie. Version 2.00.00 Int. no. 2298502,1994
04-JAN-2005 (25)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Value: = 0.839 g/cm^3

Method: calculated using Advanced Chemistry Development (ACD/Labs) Software v8.14.

GLP:

Test substance: 1-tetracosanol (506-51-4)

Reliability: (2) valid with restriction

Reference: Advanced Chemicstry Development (ACD/Labs) Software v8.14 (2006). Available at STN.

04-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Value: = 0.84 g/cm^3

Method: calculated using Advanced Chemistry Development (ACD/Labs) Software v8.14.

GLP:

Test substance: 1-hexacosanol (506-52-5)

Reliability: (2) valid with restriction

Reference: Advanced Chemicstry Development (ACD/Labs) Software v8.14 (2006). Available at STN.

04-APR-2007

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Value: = 0.841 g/cm^3

Method: calculated using Advanced Chemistry Development (ACD/Labs) Software v8.14.

GLP:

Test substance: 1-octacosanol (557-61-9)

Reliability: (2) valid with restriction

Reference: Advanced Chemicstry Development (ACD/Labs) Software v8.14 (2006). Available at STN.

04-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Value: = 0.841 g/cm^3

Method: calculated using Advanced Chemistry Development (ACD/Labs) Software v8.14.

GLP:

Test substance: 1-triacontanol

Reliability: (2) valid with restriction
Reference: Advanced Chemicstry Development (ACD/Labs) Software v8.14 (2006). Available at STN.
04-APR-2007

2.4 Vapour Pressure

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Value	= 57.26 hPa at 19.6 degree C
Decomposition	no
Method	other (measured)
Year	1970
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Comparative ebulliometry. The apparatus used is described in detail in one of the references along with a detailed description of its operation. The two boilers (reference plus test substance) are connected by a common pressure line. Platinum resistance thermometers are used to measure the temperature using a Mueller bridge. Water was used as the reference substance. The method is reported to be repeatable to within a few thousandths of a degree. The substance was first boiled at a pressure of around 15kN/m^2 to check for consistency in boiling temperature.
Result	Multiple measurements of vapour pressure at temperatures between approximately 20 degree C and 93 degree C (i.e. above the boiling point).
Test substance	Samples purified before use, including drying in vapour phase. Fraction molarity purity 0.9995
Reliability	(2) valid with restrictions Whilst old and not to an OECD protocol, the method and technique is well reported.
Flag	Critical study for SIDS endpoint
Reference	Ambrose D (1968), Improved boilers for the ebulliometric determination of vapour pressures, J Sci Instrum (J Physics E), series 2, vol 1, p41 Ambrose D, Sprake CHS (1970), Thermodynamic properties of organic oxygen compounds. XXV. Vapour pressures and normal boiling temperatures of aliphatic alcohols. J Chem Thermodynam, 2, 631-45
11.11.2004	(27) (28)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Value	= 78.7 hPa at 25 degree C
Decomposition	
Method	other (measured)
Year	1948

GLP	no data
Test substance	other TS: Commercial absolute
Method	Scatchard equilibrium still. Ethanol was fractionated in a 5 foot column packed with glass helices and then treated with magnesium ethylate. The final product of d^{25}_{4} 0.78506 was kept under its own vapour pressure in a sealed container over magnesium ethylate and samples were withdrawn by vacuum distillation. Vapour pressure was measured using an inverted U-tube manometer and 12 mm diameter tubing read with a M901 Gaertner cathetometer at a distance of 250 m. Static measurements were made by vapour pressure cell connected directly to the manometer. Agreement between methods was within 0.2 mmHg.
Result	Value was recorded as 59.03 mmHg and converted.
Source	U.S. Environment Protection Agency High Production Volume, Chemical Right to Know Program.
Reliability	(2) valid with restrictions
Reference	Howard, P. (1990). Handbook of Environmental Fate and Exposure Data for Organic Chemicals, volume II. Solvents, Lewis Publishers: Chelsea, MI.
11.11.2004	(35)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Value	= 66.3 hPa at 21.2 degree C
Decomposition	
Method	other (measured): see remark
Year	
GLP	
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Test performed at Sheffield Hallam university using and isoteniscope and internal method QP58
Result	Vapour pressure 76.0 hPa @ 24.4 deg C
Reliability	(2) valid with restrictions
Reference	BP Chemicals Ltd. Internal data 1997, 1998 and 1999.
11.11.2004	(30)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Value	66.66 hPa at 25 °C
Decomposition	

Method	other (measured)
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Method not specified.
Reliability	(4) not assignable
Reference	International Critical Tables of Numerical Data, Physics, Chemistry and Technology, Vol. III, McGraw-Hill, New York, 1928.
11.11.2004	(36)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Value	= 18 psi at 38°C
Decomposition	
Method	
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Value is Reid vapour pressure in psi.
Reliability	(4) not assignable
Reference	Kavanaugh, M.C; , Stocking, A. (1999). Fate and Transport of Ethanol in the Environment. US EPA Blue Ribbon Panel. URL http://www.epa.gov/oar/caaac/mtbeethan.pdf.
11.11.2004	(37)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Value	= 49 - 56 mm Hg
Decomposition	
Method	
Year	1999
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Value is mmHg.
Reliability	(4) not assignable
Reference	Kavanaugh, M.C; , Stocking, A. (1999). Fate and Transport of Ethanol in the Environment. US EPA Blue Ribbon Panel. URL http://www.epa.gov/oar/caaac/mtbeethan.pdf.
11.11.2004	(37)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Value	= 179.35 hPa at 40 degree C

Decomposition	no
Method	other (measured)
Year	1979
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Method designed to pressure isotherm data for binary mixtures. Temperatures measured to 0.01 degree C.
Reliability	(4) not assignable
Reference	Maher PJ, Smith BD (1979) A new total pressure vapor-liquid equilibrium apparatus. The ethanol+aniline system at 313.15, 350.81 and 386.67 K. J Chem Eng Data, 24, 1, p. 16-22
11.11.2004	(38)

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Preferred Value

Value:	0.56 hPa at 20°C
Method:	Method not listed.
GLP:	no
Test substance:	99.9% 1-butanol (71-36-3)
Comments:	As cited in Chemical Manufacturers Association. Summary of Responses to the OECD Request for Available Data on HVP Chemicals. February 8, 1999.
Reliability:	(2) valid with restrictions, full experimental data not available.
Reference:	Union Carbide Corporation. 1992a. Material Safety Data Sheet. Dated March 20, 1992. C0269D. Solvents and Coatings Materials Division, Union Carbide Corporation.

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Value:	0.658 hPa (0.49 mm Hg) at 20°C
Method:	Calculated
GLP:	no
Test substance:	99.9% 1-butanol (71-36-3)
Reliability:	(2) valid with restrictions, full experimental data not available
Reference:	Munday, E.B. Mullins, I.C. and Edie, D.D. 1980. Vapor pressure data for toluene, 1-pentanol, 1-butanol, water and 1-propanol. K. Chem Eng Data 25: 191-4

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Value:	0.82 kPa at 25°C
Method:	method not listed
GLP:	no
Test substance:	99.9% 1-butanol (71-36-3)

Reliability: (2) valid with restrictions, full experimental data not available
Reference: Bernstein a.E III, 2; b. E IV 1/3.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Value: 8.70 hPa (6.47 mm Hg) at 20°C
Method: calculated
GLP: no
Test substance: 99.9% 1-butanol (71-36-3)
Reliability: (2) valid with restrictions, full experimental data not available
Reference: Boublik, T. V Fried, and E. Hala. 1984. The vapor pressure of pure substances: selected values of the temperature dependence of the vapor pressures of some pure substances in the normal and low temperature regions. Vol. 17. Elsevier Science Publishers, Amsterdam, Netherlands.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Value: 9.36 hPa (7.024 mm Hg) at 20°C
Method: calculated
GLP: no
Test substance: 99.9% 1-butanol (71-36-3)
Reliability: (2) valid with restrictions, full experimental data not available
Reference: Howard, P .H. 1990. Handbook of Environmental Fate and Exposure Data for Organic Chemicals, Volume II. Lewis Publishers, Chelsea MI.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 1.22 hPa at 25 degree C

Method: other (measured)
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
Flag: Critical study for SIDS endpoint
Reference: Daubert, T.E. and Danner, R.P. 1989. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis.
11-OCT-2005 (18)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 1.21 hPa at 25 degree C

Method: other (calculated): from composition
Year: 2005
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Remark: For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
Reliability: (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
11-OCT-2005 (1)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 1 hPa at 20 degree C

GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Material Safety Data Sheets, NACOL 6-97 and NACOL 6M, Condea Chemie GmbH, Version 1.00.02, Int. no. 699003, 1994.
11-OCT-2005 (35)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 1.3 hPa at 20 degree C

Method: other (calculated)
Test substance: >95% 1-hexanol (111-27-3)

Reliability: (4) not assignable
Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.

11-OCT-2005 (77)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: ca. 2 hPa at 40 degree C

GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Source: Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: MSDS Henkel KGaA. Lorol C 6 (DED 00003640 00, Ausgabe 01 vom 21.04.1994)
11-OCT-2005 (40)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 0.1 hPa at 25 degree C

Method: other (measured)
Test substance: > 90% 1-octanol (111-87-5)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
Flag: Critical study for SIDS endpoint
Reference: Daubert, T.E. and Danner, R.P. 1989. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis.
03-JAN-2005 (37)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 1.3 hPa at 54 degree C

Test substance: > 90% 1-octanol (111-87-5)

Reliability: (4) not assignable
Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley &

Sons, Inc.
03-JAN-2005 (122)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 0.031 hPa at 20 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Chemical Safety Sheets: Working safely with hazardous chemicals" Kluwer Academic Publishers, 1991.
03-JAN-2005 (34)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 1.33 at 54 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Lide, D.R. (ed.), "CRC Handbook of Chemistry and Physics", 71st edition, CRC Press, Boca Raton (1990-1991).
03-JAN-2005 (76)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 2.2 hPa at 60.1 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference cited is an authoritative, peer-reviewed secondary data source (Beilstein).

Reference: Beilstein ONLINE
03-JAN-2005 (17)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 50.64 hPa at 113.3 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Boublik,T. et al., "The Vapour Pressures of Pure Substances", Elsevier Scientific Publishing Company, Amsterdam (1973)
03-JAN-2005 (21)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: 0.11 hPa at 25 degree C

Method: other (calculated): from composition
Year: 2005
GLP: no
Test substance: > 90% 1-octanol (111-87-5)

Remark: For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis
Reliability: (2) valid with restrictions
Valid with restrictions.
The value was predicted using a partial vapour pressure contribution method, supported by additional validation
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
09-AUG-2005 (3)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 0.0113 hPa at 25 degree C

Test substance: > 90% 1-decanol (112-30-1)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
Flag: Critical study for SIDS endpoint
Reference: Daubert, T.E. and Danner, R.P. 1989. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis.
05-OCT-2005 (22)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 2.93 hPa at 91 degree C

Test substance: > 90% 1-decanol (112-30-1)

Reliability: (4) not assignable
Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.
03-JAN-2005 (100)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 1.33 hPa at 69.5 degree C

Test substance: > 90% 1-decanol (112-30-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Lide, D.R. (ed.), "CRC Handbook of Chemistry and Physics", 71st edition, CRC Press, Boca Raton (1990-1991).
03-JAN-2005 (61)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 293 at 90.9 degree C

Test substance: > 90% 1-decanol (112-30-1)

Source: Henkel KGaA Duesseldorf
Reliability: (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference cited is an authoritative, peer-reviewed secondary data source
Reference: Beilstein ONLINE.
03-JAN-2005 (14)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 0.012 hPa at 25 degree C

Method: other (calculated): from composition
Year: 2005
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Remark: For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
Reliability: (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
09-AUG-2005 (2)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Value: = 0.00113 hPa at 25 degree C

Method: other (measured)
Test substance: dodecanol (112-53-8)

Source: Daubert and Danner 1989.
Reliability: (2) valid with restrictions
Reference: Daubert, T.E. and Danner, R.P. 1989. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis.
30-SEP-2003 (4)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Value: = 0.0087 hPa at 20 degree C

Test substance: dodecanol (112-53-8)
Source: Verschueren 1996.
Reliability: (4) not assignable
Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.
30-SEP-2003 (25)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 0.00014 hPa at 25 degree C

Test substance: > 95% 1-tetradecanol (112-72-1)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
Flag: Critical study for SIDS endpoint
Reference: Daubert, T.E. and Danner, R.P. 1989. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis.
04-JAN-2005 (14)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 0.0133 at 20 degree C

Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Sax, N.I. & Lewis, R.J., Hawley"s condensed chemical dictionary, 11th ed, Van Nostrand Reinhold Co., New York (1987)
04-JAN-2005 (61)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 0.00015 hPa at 25 degree C

Method: other (calculated): from composition

Year: 2005
GLP: no
Test substance: > 95% 1-Tetradecanol (112-72-1)

Remark: For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
Reliability: (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
09-AUG-2005 (3)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 0.000014 hPa at 25 degree C

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
Flag: Critical study for SIDS endpoint
Reference: Daubert, T.E. and Danner, R.P. 1989. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis.
04-JAN-2005 (18)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 1.3 hPa at 123 degree C

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Reliability: (4) not assignable
Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.
04-JAN-2005 (95)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 0.00000407 hPa at 30 degree C

Method: other (measured)
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Reliability: (4) not assignable
Reference: Littlewood, R.; Vapor pressures of some solid organic compounds.; J. Chem. Soc. pp.2419-20.; 1957. Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.
04-JAN-2005 (55) (85)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 1.33 hPa at 122.7 degree C

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The cited reference is a recognised source of physico-chemical data.
Reference: Lide, D.R. (ed.), "CRC Handbook of Chemistry and Physics", 71st edition, CRC Press, Boca Raton (1990-1991)
04-JAN-2005 (53)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 0.000016 at 25 degree C

Method: other (calculated): from composition
Year: 2005
GLP: no
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
Reliability: (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
09-AUG-2005 (3)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Value: = 0.0000033 hPa at 25 degree C

Method: other (measured)
Test substance: octadecanol (112-92-5)

Source: Daubert and Danner 1989.
Reliability: (2) valid with restrictions
Reference: Daubert, T.E. and Danner, R.P. 1989. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis.
01-OCT-2003 (2)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Value: = 1.33 hPa at 150.3 degree C

Test substance: octadecanol (112-92-5)

Source: SIDS Dossier on 1-octadecanol 1993b.
Reliability: (2) valid with restrictions
Reference: SIDS Dossier on 1-octadecanol. 1993b. Environmental Protection Agency, Denmark. 6 June 1993.
01-OCT-2003 (12)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Value: = 0.00000015 hPa at 25 degree C

Test substance: >= 90% 1-eicosanol (629-96-9)

Source:
Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
Flag: Critical study for SIDS endpoint
Reference: Daubert and Danner 1989.
04-JAN-2005

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Value: < 1 hPa at 20 degree C

GLP: no

Test substance: >= 90% 1-eicosanol (629-96-9)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Material Safety Data Sheets, NACOL 20-95 and NACOL 20-96, Condea Chemie GmbH, 1994.
04-JAN-2005 (15)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Value: =0.00000016 hPa at 25 degree C

Method: other (calculated): from composition
Year: 2005
GLP: no
Test substance: >= 90% 1-eicosanol (629-96-9)

Result: Result = 1.6×10^{-7} hPa
Reliability: (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
19-SEP-2005 (1)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Value: = .000000082 hPa at 25 degree C

Method: other (calculated): from composition
Year: 2005
GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Remark: For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
Result: Result = 8.2×10^{-8} hPa
Reliability: (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.

Flag: Critical study for SIDS endpoint
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
11-OCT-2005 (1)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Value: < 1 hPa at 20 degree C

GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source (secondary literature) to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: NACOL 22-98 Material Safety Data Sheet. RWE-DEA AG fur Mineraloel und Chemie. Version 2.00.00 Int. no. 2298502,1994
11-OCT-2005 (25)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Value: = 2.4 x 10^{-9} mm Hg 25 degree C

Method: other: calculated (SRC MPBPVP v1.41)
Year: 2007
GLP: no
Test substance: 1-tetracosanol (506-51-4)

Remark: The presence of branched components in the substance, within is expected to raise the boiling point of those substances slightly, though it is not possible to predict values precisely. Validation of boiling point prediction using this method shows that the calculated values are very close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: SRC MPBPVP v1.41. US EPA, 2006.
04-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Value: = 2.16 x 10^{-9} mm Hg at 25 degree C

Method: other: calculated (SRC MPBPVP v1.41)
Year: 2007
GLP: no
Test substance: 1-hexacosanol (506-52-5)

Remark: The presence of branched components in the substance, within is expected to raise the boiling point of those substances slightly, though it is not possible to predict values precisely. Validation of boiling point prediction using this method shows that the calculated values are very close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: SRC MPBPVP v1.41. US EPA, 2006.
04-APR-2007

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Value: = 4.02 x 10-10 mm Hg at 25 degree C

Method: other: calculated (SRC MPBPVP v1.41)
Year: 2007
GLP: no
Test substance: 1-octacosanol (661-19-8)

Remark: The presence of branched components in the substance, within is expected to raise the boiling point of those substances slightly, though it is not possible to predict values precisely. Validation of boiling point prediction using this method shows that the calculated values are very close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: SRC MPBPVP v1.41. US EPA, 2006.
04-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Value: = 7.1 x 10^{-11} mm Hg at 25 degree C

Method: other: calculated (SRC MPBPVP v1.41)
Year: 2007
GLP: no
Test substance: 1-triacontanol

Remark: The presence of branched components in the substance, within is expected to raise the boiling point of those substances slightly, though it is not possible to predict values precisely. Validation of boiling point prediction using this method shows that the calculated values are very close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: SRC MPBPVP v1.41. US EPA, 2006.
04-APR-2007

2.5 Partition Coefficient

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Partition coefficient	octanol-water
Log Pow	= -.31 at 25 °C
pH value	
Method	other (measured)
Year	1985
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Test method and date are not known.
Reliability	There is no mention of surface activity, dissociative properties, or of water solubility. (2) valid with restrictions This value has been accepted by U.S. Environment Protection Agency High Production Volume, Chemical Right to Know Program.
Flag	Critical study for SIDS endpoint
Reference	Howard, P. (1990). Handbook of Environmental Fate and Exposure Data for Organic Chemicals, volume II. Solvents, Lewis Publishers: Chelsea, MI.
05.10.2003	(35)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Partition coefficient	octanol-water
Log Pow	= -.16 to -.32
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Value expressed as log Kow and presumed calculated.
Reliability	(4) not assignable Secondary source
Reference	Kavanaugh, M.C; Stocking, A. (1999). Fate and Transport of Ethanol in the Environment. US EPA Blue Ribbon Panel. URL http://www.epa.gov/oar/caaaclmtbeethan.pdf.
29.09.2003	(40)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Partition coefficient	octanol-water
Log Pow	= -.32 at 25°C
pH value	
Method	No details of method available.
Year	
GLP	
Test substance	95 – 99.9% ethanol (64-17-5)
Reliability	(4) not assignable
Reference	Verschueren, K. Handbook of environmental data on organic chemicals. 3rd Edition. Van Nostrand Reinhold Company, New York.
05.10.2003	(41)

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Preferred Value	
Value:	log Kow = 0.88 at 20°C
Method:	Measured
GLP:	No
Test substance:	99.9% 1-butanol (71-36-3)
Analytical Method:	Internal Union Carbide
Reliability:	(2) valid with restrictions, calculated
Reference:	Hansch, C. and A. J. Leo. 1985. Medchem Project. Pomona College, Issue 26, Claremont, CA.

<u>1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)</u>

Partition Coeff.: octanol-water
log Pow: = 2.03

Method: other (measured)
Test substance: >95% 1-hexanol (111-27-3)

Method: The generator column was coated with liquid solute and 1-octanol. Water was then pumped into the column. Analysis of the aqueous phase from the 1% octanol coated column was used to determine the Kow.
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Tewari, Y.B., Miller, M.M., Wasik, S.R., and Martire, D.E. 1982. Aqueous solubility and octanol/water partition coefficient of organic compounds at 25 degrees C. J. Chem. Eng. Data 27:451-454.
03-JAN-2005 (70)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

log Pow: = 3.15

Method: other (measured): No particulars on method stated.
Test substance: > 90% 1-octanol (111-87-5)

Remark: Several estimated values were presented in IUCLID 2000. The estimated values are of the same order as this measurement but are of lower reliability and are not presented here.
Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for octanol-water partition coefficient values.
Flag: Critical study for SIDS endpoint
Reference: Hansch, C. et al., Crit. Rev. Toxicol. 19, 185-226 (1989)).
03-JAN-2005 (45)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

log Pow: = 2.8

Method: other (measured): No particulars on method stated.
Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.

References: Kogai Shigen Kenkyusho Iho 11, 77-82 (1981).

Yonezawa, Y. and Urushigawa, Y. 1979. Chemico-biological interactions in biological purification systems. V. Relation between biodegradation rate constants of aliphatic alcohols by activated sludge and their partition coefficients in a 1-octanol-water system. Chemosphere 3: 139-142.

03-JAN-2005 (73) (128)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

log Pow: = 3.07

Method: other (measured): No particulars on method stated.
Test substance: > 90% 1-octanol (111-87-5)

Reliability: (4) not assignable
Value obtained from secondary literature. The original source is not stated.
Reference: Abraham MH, et al; J. Pharma. Sci. 83: 1085 - 100 (1994).

03-JAN-2005 (1)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Partition Coeff.: octanol-water
log Pow: = 4.57

Test substance: > 90% 1-decanol (112-30-1)

Reliability: (2) valid with restrictions
valid with restrictions Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for octanol-water partition coefficient values.
Flag: Critical study for SIDS endpoint
Reference: Hansch. C., A. Leo and D. Hoekman. 1995. Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Professional Reference Book. Washington, DC: American Chemical Society.

03-JAN-2005 (32)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Partition Coeff.: octanol-water
log Pow: = 5.36

Method: other (measured)
Test substance: dodecanol (112-53-8)

Method: A reverse-phase high pressure liquid chromatography/mass spectrometery method was used to estimate Kow in complex chemical mixtures.
Source: Burkhard et al. 1985.
Test condition: ambient temperature
Reliability: (2) valid with restrictions
Reference: Burkhard, L.P., Kuehl, D.W., and Veith, G.D. 1985. Evaluation of reverse phase liquid chromatography/mass spectrometry for estimation of N-octanol/water partition coefficients for organic chemicals. Chemosphere 14(10):1551-1560.
01-OCT-2003 (3)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Partition Coeff.: octanol-water
log Pow: = 5.13

Test substance: Dodecanol (112-53-8)

Method other (measured)
Source: SRC.
Reliability: (4) not assignable
Reference: Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.
01-OCT-2003 (20)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Partition Coeff.: octanol-water
log Pow: = 6.03

Method: other (measured): Reverse-phase HPLC with mass spectrometry
Test substance: > 95% 1-Tetradecanol (112-72-1)

Method: A reverse-phase high pressure liquid chromatography/mass spectrometery method was used to estimate Kow in complex chemical mixtures.
Test condition: Column: 5 µm Ultrasphere-ODS 2.0 mm i.d. x 25 cm.
Mobile Phase: Solution A: methanol:ethanol:water 70:15:15.
Solution B: methanol:ethanol:water 95:5:0
100% A for 1 min
Gradient to 100% B at 6.67% per min
100% B for 30 min. Seven reference standards were used to correlate elution time with Kow. Dead time was measured using a non-retained substance (either acetone or acetonitrile).
Reliability: (2) valid with restrictions

Test is comparable to OECD guideline with some experimental differences and was not conducted to GLP.

Flag: Critical study for SIDS endpoint

Reference: Burkhard, L.P., Kuehl, D.W., and Veith, G.D. 1985. Evaluation of reverse phase liquid chromatography/mass spectrometry for estimation of N-octanol/water partition coefficients for organic chemicals. Chemosphere 14(10):1551-1560.

04-JAN-2005 (10)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Partition Coeff.: octanol-water

log Pow: = 6.36

Method: other (measured): details of method not stated

Test substance: > 95% 1-tetradecanol (112-72-1)

Reliability: (4) not assignable

Value obtained from secondary literature. Original source not stated.

Reference: Abraham MH, et al; J. Pharma Sci 83: 1085 - 100 (1994)

04-JAN-2005 (1)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Partition Coeff.: octanol-water

log Pow: = 6.65

Method: other (measured): Reverse-phase HPLC with mass spectrometry

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: A reverse-phase high pressure liquid chromatography/mass spectrometery method was used to estimate Kow in complex chemical mixtures. Test conditions

Column: 5 µm Ultrasphere-ODS 2.0 mm i.d. x 25 cm

Mobile Phase:

Solution A: methanol:ethanol:water 70:15:15

Solution B: methanol:ethanol:water 95:5:0. 100% A for 1 min. Gradient to 100% B at 6.67% per min. 100% B for 30 min. Seven reference standards were used to correlate elution time with Kow. Dead time was measured using a non-retained substance (either acetone or acetonitrile).

Reliability: (2) valid with restrictions

Test is comparable to OECD guideline with some experimental differences and was not conducted to GLP.

Flag: Critical study for SIDS endpoint
Reference: Burkhard, L.P., Kuehl, D.W., and Veith, G.D. 1985. Evaluation of reverse phase liquid chromatography/mass spectrometry for estimation of N-octanol/water partition coefficients for organic chemicals. Chemosphere 14(10):1551-1560.
04-JAN-2005 (14)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Partition Coeff.: octanol-water
log Pow: = 7.19

Method: other (measured)
Test substance: Octadecanol (112-92-5)

Method: A reverse-phase high pressure liquid chromatography/mass spectrometery method was used to estimate Kow in complex chemical mixtures.
Source: Burkhard et al. 1985.
Reliability: (2) valid with restrictions

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Partition Coeff.: octanol-water
log Pow: = 7.75

Method: other (measured): Reverse-phase HPLC with mass spectrometry
Test substance: >= 90% 1-eicosanol (629-96-9)

Method: A reverse-phase high pressure liquid chromatography/mass spectrometery method was used to estimate Kow in complex chemical mixtures. Test conditions: Column: 5 µm Ultrasphere-ODS 2.0 mm i.d. x 25 cm. Mobile Phase:
Solution A: methanol:ethanol:water 70:15:15.
Solution B: methanol:ethanol:water 95:5:0. 100% A for 1 min.
Gradient to 100% B at 6.67% per min. 100% B for 30 min. Seven reference standards were used to correlate elution time with Kow. Dead time was measured using a non-retained substance (either acetone or acetonitrile).
Reliability: (2) valid with restrictions
Test is comparable to OECD guideline with some experimental differences and was not conducted to GLP.
Flag: Critical study for SIDS endpoint
Reference: Burkhard, L.P., Kuehl, D.W., and Veith, G.D. 1985. Evaluation of reverse phase liquid chromatography/mass spectrometry for estimation of N-octanol/water partition coefficients for organic chemicals. Chemosphere

14(10):1551-1560.
04-JAN-2005 (8)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

log Pow: = 7.75

Method: other (calculated): amended SRC KOWWIN v1.66
Year: 2004
GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Method: The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
Remark: The presence of branched components is not expected to significantly affect the predicted value.
Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
07-JAN-2005 (1)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

log Pow: = 10.6630

Method: other (calculated): amended SRC KOWWIN v1.67
Year: 2006
GLP: no
Test substance: 1-tetracosanol (506-51-4)

Method: The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
Remark: The presence of branched components is not expected to significantly affect the predicted value.

A selection of accepted prediction methods were compared and

the results were found to be in good agreement.
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: SRC KOWWIN v1.67. US EPA, 2006.
04-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

log Pow: = 11.6452

Method: other (calculated): amended SRC KOWWIN v1.67
Year: 2006
GLP: no
Test substance: 1-hexacosanol (506-52-5)

Method: The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
Remark: The presence of branched components is not expected to significantly affect the predicted value.

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: SRC KOWWIN v1.67. US EPA, 2006.
04-APR-2007

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

log Pow: = 12.6274

Method: other (calculated): amended SRC KOWWIN v1.67
Year: 2006
GLP: no
Test substance: 1-octacosanol (557-61-9)

Method: The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
Remark: The presence of branched components is not expected to significantly affect the predicted value.

A selection of accepted prediction methods were compared and the results were found to be in good agreement.

Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.

Flag: Critical study for SIDS endpoint

Reference: SRC KOWWIN v1.67. US EPA, 2006.

04-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

log Pow: = 13.6096

Method: other (calculated): amended SRC KOWWIN v1.67

Year: 2006

GLP: no

Test substance: 1-triacontanol (593-50-0)

Method: The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.

Remark: The presence of branched components is not expected to significantly affect the predicted value.

A selection of accepted prediction methods were compared and the results were found to be in good agreement.

Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.

Flag: Critical study for SIDS endpoint

Reference: SRC KOWWIN v1.67. US EPA, 2006.

04-APR-2007

2.6.1 Solubility in different media

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Solubility in	Water
Value	> 10000 mg/l at 25°C
pH	
value	= 0
concentration	
Method	Other
Year	1900
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)

Reliability	(2) valid with restrictions
Flag	Critical study for SIDS endpoint
Reference	Howard, P. (1990). Handbook of Environmental Fate and Exposure Data for Organic Chemicals, volume II. Solvents, Lewis Publishers: Chelsea, MI.
19.10.2002	(35)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Solubility in	Water
Description	Miscible
Test substance	95 – 99.9% ethanol (64-17-5)
Reliability	(2) valid with restrictions
Reference	Merck (1996) The Merck Index 12th edition, Merck & Co., Inc., Rahway, New Jersey.
16.01.2004	(26)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Solubility in	Water
Description	Miscible
Test substance	95 – 99.9% ethanol (64-17-5)
Reliability	(4) not assignable
Reference	U.S. EPA URL http://www.epa.gov/oar/caaac/mtbeethan.pdf.
19.10.2002	(42)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Solubility in	Water
pKa	0 at 25°C
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Ethanol is stable in water. pKa is irrelevant.
Reliability	(4) not assignable
Reference	CEFIC Ethyl Alcohol Group (2003).
29.09.2003	(1)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Description	Miscible
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Described as infinite solubility of ethanol in water and water in ethanol.
Source	Riddick JA, Bunger WB, Sakano TK (1986), Techniques of Chemistry, Vol II, Organic Solvents, Physical Properties and Methods

of Purification, Wiley.
Reliability (4) not assignable
Reference Doolittle AK (1935) Lacquer solvents in commercial use, Ind Eng Chem, 27, p. 1169-79.
19.10.2002 (43)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Preferred Value
Value: 77,000 mg/l at 200 degree C
Method: Not Stated
GLP: No
Test substance: 99.9% 1-butanol (71-36-3)
Reliability: (2) valid with restrictions, full experimental details not available
Reference: Howard, P;H. 1990. Handbook of Environmental Fate and Exposure Data for Organic Chemicals, Volume II. Lewis Publishers, Chelsea, MI

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Solubility in: Water
Value: = 5900 mg/l at 25 degree C

Method: other
Test substance: >95% 1-hexanol (111-27-3)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered authoritative for water solubility values.
Flag: Critical study for SIDS endpoint
Reference: Yalkowsky, S.H.; Dannenfelser, R.M.; AQUASOL database of aqueous solubility. Version 5; College of Pharmacy, University of Arizona - Tucson, AZ. PC version.; 1992
08-AUG-2005 (83)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Solubility in: Water
Value: = 4231 mg/l at 20 degree C

Method: other
Test substance: >95% 1-hexanol (111-27-3)

Method: A generator column was coated with liquid solute. Water was pumped into the column. Analysis of the aqueous phase from the pure solute coated column yielded the aqueous

solubility.
Reliability: (2) valid with restrictions
Reference: Tewari, Y.B., Miller, M.M., Wasik, S.R., and Martire, D.E. 1982. Aqueous solubility and octanol/water partition coefficient of organic compounds at 25 degrees C. J. Chem. Eng. Data 27:451-454.
03-JAN-2005 (70)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Solubility in: Water
Value: = 6 g/l at 25 degree C

GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
Reference: Material Safety Data Sheets, NACOL 6M, NACOL 6-97, NACOL 6-98, NACOL-99, Condea Chemie GMbH, Version 1.00.02, Int. no. 0699003, 1994.
03-JAN-2005 (36)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Solubility in: Water
Value: = 6270 mg/l at 25 degree C

Test substance: >95% 1-hexanol (111-27-3)

Reliability: (2) valid with restrictions
Reference: Veith, G.D., Call, D.J., and Brooke, L.T. 1983a. Estimating the acute toxicity of narcotic chemicals to fathead minnows. In: Bishop, W.E., Cardwell, R.D., and Heidolph, B.B. (eds.). Aquatic Toxicology and Hazard Assessment: Sixth Symposium. ASTM STP 802. American Society for Testing and Materials, Philadelphia.
21-SEP-2005 (75)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Solubility in: Water

Value: = 5760 mg/l at 25 degree C

Method: other: (calculated) partition model
Year: 2005
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Method: For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
Remark: Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
Result: The water solubility is estimated to be 5760 mg/l at a loading rate of 10000 mg/l.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
09-AUG-2005 (1)

<u>1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)</u>

Solubility in: Water
Value: = 551 mg/l

Test substance: > 90% 1-octanol (111-87-5)

Reliability: (2) valid with restrictions
Valid with restrictions. Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for solubility values.
Flag: Critical study for SIDS endpoint
Reference: Yalkowsky and Valvani J.Pharm Sci 69 912 (1980), cited in Satyanarayana, D.; Charyulu, R. Narayana; Nagavi, B. G., Asian Journal of Chemistry (1997), 9(3), 418-426.
03-JAN-2005 (126)

<u>1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)</u>

Solubility in: Water
Value: = 495 - 596 mg/l at 25 degree C

Method: other
Test substance: > 90% 1-octanol (111-87-5)

Reliability: (4) not assignable
Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.
03-JAN-2005 (122)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Solubility in: Water
Value: = 540 mg/l at 25 degree C

Method: other: measured
Test substance: > 90% 1-octanol (111-87-5)

Source: SRC.
Reliability: (4) not assignable
Reference: Barton, A.F.M.; Alcohols with water; International Union of Pure and Applied Chemistry. Solubility data series. vol. 15, 438, pp. 1984.
03-JAN-2005 (14)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 300 mg/l at 20 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.
05-JAN-2005 (122)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 495 mg/l at 25 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Kinoshita, K. et al., Bull. Chem. Soc. Japan 31, 1081-1082 (1958).
05-JAN-2005 (72)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 586.17 mg/l at 25 degree C

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Bell, G.H., Chem. Phys. Lipids 10, 1-10 (1973).
05-JAN-2005 (18)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Solubility in: Water
Value: = 560 mg/l at 25 degree C

Method: other: (calculated) partition model
Year: 2005
GLP: no
Test substance: > 90% 1-octanol (111-87-5)

Method: For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.

Remark: Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
Result: The water solubility is estimated to be 560 mg/l at a loading rate of 1000 mg/l.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
09-AUG-2005 (3)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Solubility in: Water
Value: = 500 mg/l at 25 degree C

Method: other: measured
Test substance: > 90% 1-octanol (111-87-5)
Reliability: (2) valid with restrictions
This information was obtained from an authoritative, peer-reviewed secondary data source (Beilstein).
Reference: Beilstein Chemical Database, 2005.
21-SEP-2005 (16)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Solubility in: Water
Value: = 39.5 mg/l

Method: other: measured
Test substance: > 90% 1-decanol (112-30-1)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for water solubility values.
Flag: Critical study for SIDS endpoint
Reference: Yalkowsky and Valvani J.Pharm Sci 69 912 (1980) cited in Satyanarayana, D.; Charyulu, R. Narayana; Nagavi, B. G., Asian Journal of Chemistry (1997), 9(3), 418-426.
03-JAN-2005 (104)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Solubility in: Water

Value: = 7.97 mg/l at 20 degree C

Method: other: measured (slow stir procedure)
Test substance: > 90% 1-decanol (112-30-1)
Reliability: (2) valid with restrictions
Reference: Letinski, DJ, MJ Connelly, DR Peterson and TF Parkerton. In press. Slow-stir water solubility measurements of selected alcohols and diesters. ExxonMobil. Chemosphere 2002.
03-JAN-2005 (60)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Solubility in: Water
Value: = 106 mg/l at 20 degree C

Method: other
Test substance: > 90% 1-decanol (112-30-1)

Reliability: (2) valid with restrictions
Reference: Tewari, Y.B., Miller, M.M., Wasik, S.R., and Martire, D.E. 1982. Aqueous solubility and octanol/water partition coefficient of organic compounds at 25 degrees C. J. Chem. Eng. Data 27:451-454.
03-JAN-2005 (88)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Solubility in: Water
Value: = 37 mg/l at 25 degree C

Method: other
Test substance: > 90% 1-decanol (112-30-1)

Reliability: (4) not assignable
Reference: Barton, A.F.M.; Alcohols with water; International Union of Pure and Applied Chemistry. Solubility data series. vol. 15, 438 pp; 1984.

Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.
03-JAN-2005 (12) (87)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Solubility in: Water
Value: = 39.5 mg/l at 25 degree C

Method: other: (calculated) partition model
Year: 2005
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Method: For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
Remark: Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
Result: The water solubility is estimated to be 39.5 mg/l at a loading rate of 1000 mg/l.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
09-AUG-2005 (2)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Solubility in: Water
Value: = 40 mg/l at 25 degree C

Test substance: > 90% 1-decanol (112-30-1)

Reliability: (2) valid with restrictions
Reference: Beilstein online Handbook of Organic Chemistry
21-SEP-2005 (13)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)</u>

Solubility in: Water
Value: = 1.7 - 2.9 mg/l

Method: other
Test substance: dodecanol (112-53-8)

Remark: Solubility in water = 1.7 mg/l @ 16 C to 2.9 mg/l @ 34 C

Source: Verschueren 1996.
Reliability: (4) not assignable
Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.
29-OCT-2003 (25)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Solubility in: Water
Value: = 1.93 mg/l at 20 degree C

Method: other: measured (slow stir procedure)
Test substance: dodecanol (112-53-8)

Source: Letinski 2002.
Reliability: (2) valid with restrictions
Reference: Letinski, DJ, MJ Connelly, DR Peterson and TF Parkerton. In press. Slow-stir water solubility measurements of selected alcohols and diesters. ExxonMobil. Chemosphere 2002.
01-OCT-2003 (13)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Solubility in: Water
Value: = 4 mg/l at 25 degree C
Method: other (measured)
Test substance: dodecanol (112-53-8)

Source: SRC.
Reliability: (4) not assignable
Reference: Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.
29-OCT-2003 (20)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Solubility in: Water
Value: = 1.9 mg/l at 25 degree C

Method: other: measured (GC)
Test substance: dodecanol (112-53-8)

Source: Veith et al.1983a.
Reliability: (2) valid with restrictions
Reference: Veith, G.D., Call, D.J., and Brooke, L.T. 1983a. Estimating the acute toxicity of narcotic chemicals to

fathead minnows. In: Bishop, W.E., Cardwell, R.D., and Heidolph, B.B. (eds.). Aquatic Toxicology and Hazard Assessment: Sixth Symposium. ASTM STP 802. American Society for Testing and Materials, Philadelphia.
01-OCT-2003 (23)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Solubility in: Water
Value: = .191 mg/l at 25 degree C

Method: other
Test substance: > 95% 1-tetradecanol (112-72-1)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered authoritative for water solubility values.
Flag: Critical study for SIDS endpoint
Reference: Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.

YALKOWSKY, SH & DANNENFELSER, RM (1992)
11-OCT-2005 (71) (84)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Solubility in: Water
Value: = 0.35 mg/l at 25 degree C

Method: other: measured (keine weiteren Angaben)
Test substance: > 95% 1-Tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. However, the source of the value is a recognised source of physico-chemical data. This reference is considered authoritative for water solubility values.
Reference: Yalkowsky, S.H. & Valvani, S.C., J. Pharm. Sci. 69, 912-922 (1980)
11-OCT-2005 (83)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Solubility in: Water
Value: = 0.31 mg/l

Method: other
Test substance: > 95% 1-tetradecanol (112-72-1)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
Reference: Lide, D.R. (ed.). 1999. CRC Handbook of Chemistry and Physics. 80th ed. Boca Raton: CRC Press.
11-OCT-2005 (46)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Solubility in: Water
Value: 0.2 mg/l at 25 degree C

Method: other: (calculated) partition model
Year: 2005
GLP: no
Test substance: > 95% 1-tetradecanol (112-72-1)

Method: For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
Remark: Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
Result: The water solubility is estimated to be 0.202 mg/l at a loading rate of 1000 mg/l.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
11-OCT-2005 (3)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Solubility in: Water
Value: = 0.013 mg/l at 25 degree C

Method: other
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for water solubility values.
Flag: Critical study for SIDS endpoint
Reference: Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.

Yalkowsky, S.H.; Dannenfelser, R.M.; AQUASOL database of aqueous solubility. Version 5; College of Pharmacy, University of Arizona - Tucson, AZ. PC version.; 1992.
04-JAN-2005 (85) (104)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Solubility in: Water
Value: = 0.03 mg/l

Method: other
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data.
Reference: Lide, D.R. (ed.). 1999. CRC Handbook of Chemistry and Physics. 80th ed. Boca Raton: CRC Press.
04-JAN-2005 (54)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 0.12 mg/l at 25 degree C

Method: other: berechnet
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Wakita, K. et al., Chem. Pharm. Bull. 34, 4663-4681 (1986).

05-JAN-2005 (97)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 0.0134 mg/l at 25 degree C

Method: other: berechnet
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Hoffmann, C.S. & Anacker, E.W., J. Chromatogr. 30, 390-396 (1967).
05-JAN-2005 (47)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = .0143 mg/l at 25 degree C

Method: other: berechnet
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: The water solubility is estimated to be 0.043 mg/l at a loading rate of 1000 mg/l.
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Amidon, G.L. et al., J. Pharm. Sci. 63, 1858-1866 (1974).
11-SEP-2005 (1)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 0.024 mg/l at 25 degree C

Method: other: gemessen (keine weiteren Angaben)
Test substance: >= 95% 1-hexadecanol (36653-82-4)
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000

CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.

Reference: Yalkowsky, S.H. & Valvani, S.C., J. Pham. Sci. 69, 912-922 (1980).

05-JAN-2005 (103)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 0.008 mg/l at 34 degree C

Method: other: gemessen ueber radioaktive Markierung

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

Reliability: (4) not assignable

This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.

Reference: Krause, F.P. & Lange, W., J. Phys. Chem. 69, 3171-3173 (1965).

05-JAN-2005 (52)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 0.0155 mg/l at 43 degree C

Method: other: gaschromatographisch gemessen

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

Reliability: (4) not assignable

This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.

Reference: Hoffmann, C.S. & Anacker, E.W., J. Chromatogr. 30, 390-396 (1967).

04-JAN-2005 (47)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Solubility in: Water

Value: = 0.043 mg/l at 25 degree C

Method: other: (calculated) partition model

Year: 2005

GLP: no

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
Remark: Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
Result: The water solubility is estimated to be 0.043 mg/l at a loading rate of 1000 mg/l.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
17-OCT-2005 (3)

<u>1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)</u>

Solubility in: Water
Value: = 0.0011 mg/l at 25 degree C

Method: other: measured
Test substance: octadecanol (112-92-5)

Remark: Reported as insoluble in Budavari 1996.
Source: SIDS Dossier on 1-Octadecanol 1993b; Budavari 1996.
Reliability: (2) valid with restrictions
Reference: Budavari, S. (ed.). 1996. Merck Index. 12th ed. Whitehouse Station: Merck Research Laboratories.

SIDS Dossier on 1-Octadecanol. 1993b. Environmental Protection Agency, Denmark. 6 June 1993.
01-OCT-2003 (1) (12)

<u>1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)</u>

Solubility in: Water
Value: = 0.0027 mg/l at 25 degree C

Method: other: (calculated) partition model
Year: 2005

GLP: no
Test substance: >= 90% 1-eicosanol (629-96-9)

Method: For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
Remark: Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
Result: The water solubility is estimated to be 0.0027 mg/l at a loading rate of 1000 mg/l.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.
05-OCT-2005 (1)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Solubility in: Water
Descr.: not soluble

Method: other
Test substance: >= 90% 1-eicosanol (629-96-9)

Reliability: (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data.
Reference: Lide, D.R. (ed.). 1999. CRC Handbook of Chemistry and Physics. 80th ed. Boca Raton: CRC Press.
05-OCT-2005 (13)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Solubility in: Water
Value: = .0027 mg/l at 25 degree C

Method: other: (calculated) partition model
Year: 2005
GLP: no

Test substance: >95% 1-docosanol (661-19-8)

Method: For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.

Remark: Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

Result: The water solubility is estimated to be 0.0027 mg/l at a loading rate of 1000 mg/l.

Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

Flag: Critical study for SIDS endpoint

Reference: Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

11-OCT-2005 (1)

1-Tetracosanol

Solubility in: water

Value: = 1.471 x 10^{-5} mg/L at 25 degree C

Method: other (calculated): WSKOW v1.41

Year: 2006

GLP: no

Test substance: 1-tetracosanol (506-51-4)

Remark: The presence of branched components is not expected to significantly affect the predicted value.

A selection of accepted prediction methods were compared and the results were found to be in good agreement.

Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.

Flag: Critical study for SIDS endpoint

Reference: WSKOW v1.41, US EPA, 2006.

04-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67095-28-6)

Solubility in: water
Value: = 1.438 x 10^{-6} mg/L at 25 degree C

Method: other (calculated): WSKOW v1.41
Year: 2006
GLP: no
Test substance: 1-hexacosanol (506-52-5)

Remark: The presence of branched components is not expected to significantly affect the predicted value.

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: WSKOW v1.41, US EPA, 2006.
04-APR-2007

1-Octacosanol

Solubility in: water
Value: = 1.398 x 10^{-7} mg/L at 25 degree C

Method: other (calculated): WSKOW v1.41
Year: 2006
GLP: no
Test substance: 1-octacosanol (557-61-9)

Remark: The presence of branched components is not expected to significantly affect the predicted value.

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: WSKOW v1.41, US EPA, 2006.

04-APR-2007

1-Triacontanol

Solubility in: water
Value: = 1.35 x 10^{-8} mg/L at 25 degree C

Method: other (calculated): WSKOW v1.41
Year: 2006
GLP: no
Test substance: 1-triacontanol (593-50-0)

Remark: The presence of branched components is not expected to significantly affect the predicted value.

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: WSKOW v1.41, US EPA, 2006.
04-APR-2007

2.7 Flash Point

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Value	= 14°C
Type	closed cup
Method	other: Abel closed cup. IP170/95 1997
Year	
GLP	
Test substance	other TS: double rectified absolute alcohol
Remark	Test performed by SG Redwood (UK) Ltd. IS09002. no Q4856
Reliability	(2) valid with restrictions
Reference	BP Chemicals Ltd. Internal data 1997,1998 and 1999.
16.10.2003	(30)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Value	= 13 degree C
Type	closed cup
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	
Reliability	(4) not assignable
Reference	Merck (1989) The Merck Index 11th edition, Merck & Co., Inc., Rahway, New Jersey.
16.10.2003	(31)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Preferred result
Value: 37° C
Remark: 98° F
Test substance: 99.9% 1-butanol (71-36-3)
Reliability: (2) valid with restrictions, full experimental data not available
Reference: NFPA. 1994. National Fire Protection Association. Fire Protection Guide to Hazardous Materials. 11th edition. NFPA. Quincy, MA.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Value: 29°C closed cup
35°C closed cup
GLP: No
Test substance: 99.9% 1-butanol (71-36-3)
Reliability: (2) valid with restrictions, full experimental data not available.
Reference: Montgomery, John H. Groundwater Chemicals (Desk Reference). 2nd Edition, 1996.
Othmer, Kirk. 3rd Edition 21 :378.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: ca. 65 degree C
Type: closed cup

Method: other: DIN 51758/ISO 2719 (According to Pensky-Martens)
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Source: Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: MSDS Henkel KGaA. Lorol C 6 (DED 00003640 00, Ausgabe 01 vom 21.04.1994.
03-JAN-2005 (40)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 60 degree C

Test substance: >95% 1-hexanol (111-27-3)

Reliability: (4) not assignable
Value obtained from secondary literature. Original reference not stated
Reference: http://chemfinder.cambridgesoft.com/
03-JAN-2005 (27)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 62 degree C
Type: open cup

Test substance: >95% 1-hexanol (111-27-3)

Reliability: (4) not assignable
Reference: Riddick J.A., Bunger W.B., Sakano T.K., (1986), Organic Solvents: Physical properties and methods of purification, Techniques of Chemistry Volume III, 4th Edition, John Wiley and Sons, New York.
03-JAN-2005 (53)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Value: = 62 degree C

Method: other: DIN 51755
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Material Safety Data Sheets, NACOL 6-97 and NACOL 6M, Condea Chemie GmbH, Version 1.00.02, Int. no. 699003, 1994)
03-JAN-2005 (35)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: ca. 90 degree C
Type: closed cup

Method: other: DIN 51758

Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Safety data sheet Henkel KGaA
11-OCT-2005 (95)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 81 degree C

Test substance: > 90% 1-octanol (111-87-5)

Reliability: (4) not assignable
Value obtained from secondary literature.
Reference: http://chemfinder.cambridgesoft.com/
11-OCT-2005 (56)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Value: = 81 degree C
Type: other

Method: other: no information on method provided.
Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: **"**Chemical Safety Sheets: Working safely with hazardous Chemicals" Kluwer Academic Publishers, 1991.
11-OCT-2005 (34)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: = 82 degree C

Test substance: > 90% 1-decanol (112-30-1)

Remark: Although not stated, this is considered likely to be a result from a closed-cup test by comparison with other values.
Reliability: (4) not assignable
Value obtained from secondary literature. Original reference not stated.
Reference: Value obtained from the Chemfinder website at http://chemfinder.cambridgesoft.com/
03-JAN-2005 (96)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: ca. 110 degree C
Type: open cup

Method: other: DIN ISO 2592
Test substance: > 90% 1-decanol (112-30-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Safety data sheet, Henkel KgaA
03-JAN-2005 (75)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Value: ca. 110 degree C
Type: open cup

Method: other: DIN 51758
Test substance: > 90% 1-decanol (112-30-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Safety data sheet, Henkel KgaA
03-JAN-2005 (75)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

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1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: = 140 degree C

Test substance: > 95% 1-tetradecanol (112-72-1)

Remark: Whilst not stated, it is considered likely that this is a result from a closed-cup test, by comparison with other measured values.
Reliability: (4) not assignable
This value was obtained from secondary literature.
Reference: http://chemfinder.cambridgesoft.com/
04-JAN-2005 (40)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Value: ca. 155 degree C
Type: open cup

Method: other: DIN 51758/ISO 2719
Test substance: > 95% 1-tetradecanol (112-72-1)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
Reference: Safety data sheet Henkel KgaA
04-JAN-2005 (59)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: = 135 degree C

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: while not stated, it is considered likely that this is a value obtained in a closed cup test by comparison with other measured data.
Reliability: (4) not assignable
Value obtained from secondary literature. Original reference not stated.
Reference: http://chemfinder.cambridgesoft.com/
04-JAN-2005 (48)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Value: ca. 175 degree C
Type: open cup

Method: other
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Source:
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.
Reference: UNION DERIVAN S.A. VILADECANS
04-JAN-2005

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Value: = 170 degree C

Test substance: Octadecanol (112-92-5)

Source: SIDS Dossier on 1-octadecanol 1993b.
Reliability: (2) valid with restrictions
Reference: SIDS Dossier on 1-Octadecanol. 1993b. Environmental Protection Agency, Denmark. 6 June 1993.
19-AUG-2003 (12)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Value: = 195 degree C

Method: other: DIN 51758
GLP: no
Test substance: >= 90% 1-eicosanol (629-96-9)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
Reference: Material Safety Data Sheets, NACOL 20-95 and NACOL 20-96, Condea Chemie GmbH, 1994
04-JAN-2005 (15)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Value: = 195 degree C
Type: open cup

Method: other: DIN 51758
GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Since it is based on company product data which cannot be validated further, review of the original source would not alter the reliability of these data.
Reference: Material Safety Data Sheet, NACOL 22-97, Condea Chemie GmbH, 1991.
04-JAN-2005 (21)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Value: ca. 227 degree C
Type: open cup

Method: other: ISO 2592
GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Since it is based on company product data which cannot be validated further, review of the original source would not alter the reliability of these data.
Reference: NACOL 22-98 Material Safety Data Sheet. RWE-DEA AG fur Mineraloel und Chemie. Version 2.00.00 Int. no. 2298502,1994.
04-JAN-2005 (25)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Value: = 141.7 degree C

Method: calculated using Advanced Chemistry Development (ACD/Labs) Software v8.14.
GLP:
Test substance: 1-tetracosanol (506-51-4)

Reliability: (2) valid with restriction
Reference: Advanced Chemicstry Development (ACD/Labs) Software v8.14 (2006). Available at STN.
04-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Value: = 139.2 degree C

Method: calculated using Advanced Chemistry Development (ACD/Labs) Software v8.14.
GLP:
Test substance: 1-hexacosanol (506-52-5)
Reliability: (2) valid with restriction
Reference: Advanced Chemicstry Development (ACD/Labs) Software v8.14 (2006). Available at STN.
04-APR-2007

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Value: = 135.3 degree C

Method: calculated using Advanced Chemistry Development (ACD/Labs) Software v8.14.
GLP:
Test substance: 1-octacosanol (557-61-9)

Reliability: (2) valid with restriction
Reference: Advanced Chemicstry Development (ACD/Labs) Software v8.14 (2006). Available at STN.
04-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Value: = 130.1 degree C

Method: calculated using Advanced Chemistry Development (ACD/Labs) Software v8.14.
GLP:
Test substance: 1-triacontanol (593-50-0)

Reliability: (2) valid with restriction
Reference: Advanced Chemicstry Development (ACD/Labs) Software v8.14 (2006). Available at STN.
04-APR-2007

2.8 Autoflammability

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Value:	365°C
Test substance:	99.9% 1-butanol (71-36-3)
Reference:	Othmer, Kirk. 3rd Edition. 21:378

2.12 Viscosity

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Test type	other: not specified
Test procedure	
Value	= 1.22 mPa*s (dynamic) at 20°C
Result	
Method	other: IP71 1/97
Year	1997
GLP	
Test substance	other TS: double rectified absolute alcohol
Remark	Test performed by 8G Redwood {UK} Ltd. 1809002, no. Q4856.
Reliability	(2) valid with restrictions
Reference	BP Chemicals Ltd. Internal data 1997, 1998 and 1999.
29.09.2003	(30)

3.1.1 Photodegradation

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Air
Light source	Other
Light spectrum	ca. 345 - 355 nm
Relative intensity	based on intensity of sunlight
Conc. of substance	2 mg/l at 30°C
INDIRECT PHOTOLYSIS	
Sensitizer	other: NOx
Conc. of sensitizer	1 mg/L
Rate constant	= .045 cm^3/(molecule*sec)
Degradation	= 20 % after 5 hour(s)
Deg. product	
Method	other (measured): Photodegradation Test
Year	1977
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)

Method	Light source: UV fluorescent lamps. Analytical methods: GC and UV spectroscopy. Controls: unclear. Light intensity 700 muW/cm^2. Ethanol was irradiated for 5 - 6 hours in a 12 cubic metre "smog chamber" at 55% relative humidity. The amount of ethanol present was measured by GC.
Result	Indirect photolysis; t1/2 15.4 hours. % degradation results other than halflife: A 20% decrease in ethanol concentration was observed after 2 hr. Rate constant calculated (1st Order assumed) 0.045 hr^{-1} and half life 15.4 h. Ethanol ranked low on authors reactivity scale. NO depletion rate: 2.3 ppb/min
Reliability	(2) valid with restrictions No data on hydroxy radical concentrations given.
Flag	Critical study for SIDS endpoint
Reference	Yanagihara S, Shimada I, Shinoyama E, Chisaka E, Saito K. (1977) Photochemical reactivities of hydrocarbons. Proc.4th Int. Clean Air Congr. 472 - 477. (See http://esc.syrres.com/efdb/Chemfate.htm)
19.10.2004	(47)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Air
Light source	other: High pressure mercury lamp with water cooled pyrex filter > 290
Light spectrum	nm = 125 based on intensity of sunlight lambda (max, >295nm) : 182 nm
Relative intensity	epsilon (max) epsilon (295) at 25°C
Conc. of substance	
INDIRECT PHOTOLYSIS	
Sensitizer	other: O2, NOx, water
Method	other (measured)
Year	1978
GLP	no data
Test substance	other TS: analytically pure ethanol (64-17-5)
Method	Ethanol was irradiated in a 4 litre or 20 litre reactor in the presence of corresponding amounts of water, nitrogen dioxide and sulphur dioxide in synthetic air. The test concentrations used were 100, 500 and 1000 ppm (mg/l). Irradiation was for up to 10 hours. Samples were taken for analysis every hour and the reduction in ethanol concentration was measured by GC. light intensity 125W; 25-30 degree C; samples were taken hourly. Concentration of substance: 100, 500, 1000 ppm.

	Relative intensity in Watts relative to sunlight. Original paper in German.
Result	No degradation of ethanol occurred in the presence of oxygen after irradiation at >290 nm, but degradation was evident at >230 nm. After irradiation for 4 hours in the presence of nitrogen dioxide, 30% degradation occurred at 100 ppm, 55% at 500 ppm and 80% at 1000 ppm. Half life calculated to be 13.8 hours. No degradation was seen in the presence of water at >290 nm. Ethanol is not degraded in the troposphere by photodegradation in the absence of sensitisers to promote indirect degradation.
Reliability	(2) valid with restrictions No data on hydroxy radical concentrations given. No data available on concentration of sensitisers used.
Reference	Hustert, K., Mansour, M., Korte, F. (1978) Reaktionen von essigester und aethanof in gegenwart von umweltkontaminanten (NO2 und SO2) unter simulierten troposphaerischen bedingungen. Chemosphere 1, 35 - 50.
19.10.2004	(48)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Air
INDIRECT PHOTOLYSIS	
Sensitizer	OH
Conc. of sensitizer	
Rate constant	= .0000018 cm^3/(molecule/sec)
Degradation	
Deg. product	
Method	other (calculated)
Year	1976
GLP	no data
Test substance	ethanol (64-17-5)
Method	A values for the half-life in a typical urban sunlit atmosphere was calculated from the rate constant for the reaction of the hydroxyl radical with ethanol vapour, assuming hydroxyl radical concentrations in such atmospheres to the of the order of 10E-14 mol*dm-3. The calculated half-life was 10 hours.
Result	The rate constant was 1.8 +/- 0.2 x 10^-9 dm^3mol^-1 s^-1 Hydroxyl radicals were generated in a reaction vessel in a "dark system" by chain reaction in a hydrogen peroxide/nitrogen dioxide/carbon monoxide substrate mixture. No light source is used in this system.

Reliability (2) valid with restrictions No detailed methodology provided.
Reference Campball, I.M. et al. (1976) Rate constants for reactions of hydroxyl radicals with alcohol vapours at 292 K. Chem. Phys. Letters 38, 362 - 364.
19.10.2004 (49)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type Air

Test substance ethanol (64-17-5)
Remark This is a critical review of the available photodegradation data. Values quoted are:

Conclusion Rate constant k (E-12 cm3.mol-1.s-1)[temperature (K)]
3.2+/-0.4 [292] Campbell et al
3.74+/-0.37 [296+/-2] Overend et al
2.62+/-0.36 [298] Ravishankara et al
3.5+/-0.6 [295+/-2] Cox et al
2.07 [300] Meier et al
3.0 +/-0.6 [298] Lorenz et al
3.66 +/-0.42 [303+/-2] Kerr et al
3.4 +/-0.17 [293] Grenhill et al
3.33 +/-0.23 [296] Wallington et al
3.26 +/-0.14 [293] Hess et al
Following a critical review of the available data, the author concluded that the study by Hess et al (1988) was the preferred value for recommendation. This study measured rate constants over the temperature range 293-750K. An overall rate constant was calculated from the Hess data using a unit weighted least squares regression, yielding a rate constant of 3.27E-12 at 298K with an estimated uncertainty of +/-20%.
Reliability (2) valid with restrictions Whilst this is a secondary source, the data within it are critically evaluated.
The data reviewed presents a consistent picture and a weight of evidence approach also confirms the conclusions reached.
Reference Atkinson R (1989), "Kinetics and Mechanisms of the Gas-Phase reactions of the hydroxyl radical with organic compounds", J Phys Chem ref data, Monograph no 1, pub Am Chem Soc.
18.10.2004 (50)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type Air
Method other (calculated)
Year 2000

GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	SAPRG-99 chemical mechanism linked with EKMA box model descriptions of air pollution episodes in 39 urban locations. The EKMA approach involves use of single-cell box models to simulate how ozone formation in one day episodes is affected by changes in VOC and NOx inputs. Such single-cell models cannot represent realistic pollution episodes in great detail but they can represent dynamic injection of pollutants, time-varying changes of inversion heights with entrainment of pollutants from aloft as the inversion height increases throughout the day, and time varying photolysis rates, temperatures, and humidities. Thus, they can be used to simulate a wide range of the chemical conditions which affect ozone formation from reactive VOCs and NOx. These are the same as those affecting VOC reactivity, The incremental reactivity is the change in ozone formed caused by adding, in this case, ethanol to the initial and emitted base reactive organic gas mixture in a scenario, divided by the amount of VOC added.
Remark	Type: VOC reactivity scale. This is an update of the SPARC-90 mechanism of Carter (1990) and incorporates recent reactivity data on the Maximum Incremental Reactivity (MIR) Scale from a wide variety of VOCs.
Result	Absolute Value: 1.34 - 1.69 gm ozone/g VOC
Reliability	(4) not assignable
Reference	Carter, PL (1994) Development of ozone reactivity scales for volatile organic compounts. J Air Waste Man Assoc, 44, 881-899. Carter, W.P.L., The SAPRC-99 Chemical Mechanism and Updated VOC Reactivity Scales (2000). URL http://www.cert.ucr.edu/-carter/reactdat.htm
18.10.2004	(51) (52)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Air
Light source	
Light spectrum	
Relative intensity	based on intensity of sunlight
Conc. of substance	
Deg. product	yes
Method	other (calculated)
Year	2000
GLP	no data

Test substance	95 – 99.9% ethanol (64-17-5)
Method	Calculated using the Harwell Photochemical Trajectory Model using the updated IVL photochemical scheme, updated using the oxidation mechanism of the acetates, as described in the Master Chemical Mechanism oxidation mechanism. The model follows chemical development in air parcels as they travel across from continental Europe to the UK. Parcel dimensions are 10km squares to the top of the boundary layer, the latter being 300m at 06:00 rising to 1300m by 14:00, falling from early evening back to 300m. The chemical inventory of the parcel is stated in the reference (95 hydrocarbons plus methane.) The model contains 771 thermal chemical reactions, with rate constants obtained from Atkinson (1989, 1990, 1992, 1994) or calculated using SAR (Atkinson(1986, 1987).
Remark	Type: Tropospheric ozone creation potential.
Result	The photochemical ozone creation potential (POCP) concept can be regarded as useful in locations with high NOx concentrations where the rate limiting step in ozone creation is the VOC composition and reactivity. Photochemical Ozone creation potential 39.9% (Andersson-Skold) or 44.6 (Derwent) relative to ethylene at 100%, with ethanol representing 4.28% of total VOC emissions. POCP figures are considered to be to an accuracy 01+/-5. Ethanol is considered to degrade by reaction with OH radicals and via carbon/carbon scission.
Reliability	(4) not assignable
Reference	Andersson-Skold, Y. and L. Holmberg. (2000) "Photochemical Ozone Creation Potentials (POCP) and Replacement of Solvents in Europe". Atmospheric Environment 34:3159-3169. Derwent RG,Jenkin, ME, Saunders SM (1996). Photochemical ozone creation potentials for a large number of reactive hydrocarbons under European conditions. Atmosp. Env 30, 2, p. 181.
18.10.2004	(53) (54)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Air
DIRECT PHOTOLYSIS	= 3 day(s)
Halflife t1/2	
Degradation	% after
Quantum yield	
INDIRECT PHOTOLYSIS	
Sensitizer	
Conc. of sensitizer	
Rate constant	0.0000000000035763 cm^3/(molecule*sec)

Degradation	% after
Deg. product	
Method	other (calculated)
Year	
GLP	
Test substance	ethanol (64-17-5)
Remark	Note: Half life based on 12 hour day. Calculated value.
Result	SUMMARY (AOP v1.90): HYDROXYL RADICALS Hydrogen Abstraction = 3.4363 E-12 cm3/mol-sec Reaction with N, Sand -OH = 0.1400 E-12 cm3/mol-sec Addition to Triple Bonds = 0.0000 E-12 cm3/mol-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/mol-sec Addition to Aromatic Rings = 0.0000 E-12 cm3/mol-sec Addition to Fused Rings = 0.0000 E-12 cm3/mol-sec OVERALL OH Rate Constant = 3.5763 E-12 cm3/mol-sec
Reliability	(2) valid with restrictions
Reference	US Environmental Protection Agency (2000).
12.11.2004	(45)

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Preferred Value	
Type:	Other, see remarks
Light Source:	
Light spect.:	
Rel. intensity:	based on intensity of sunlight
Degradation:	30 hour half-life
Method:	
GLP:	
Test substance:	butanol
Remark:	Atmospheric photo-oxidation potential was. estimated using a measured or estimated second order half-life with units of cm3/molecules-cm reported by Kwok and Atkinson (1994). Vapor phase butanol is expected to degrade in the atmosphere by reaction with photochemically produced hydroxyl (OH) radicals. The 2nd order rate constant was reported to be 8.57 e-12 cm3 (molecule/see) at 25°C. Based on 1.5E6 OH molecules/cm3 and assuming 12 hours of sunlight per day, the estimated half-life was 1.25 days or 30 hours.
Reliability:	(2) valid with restrictions, full experimental data not available
Reference:	Kwok and Atkinson (1994) as reported in AOPWIN version J .90. Atmospheric Oxidation. EPIWIN (Estimation Program Interface for

Windows) version 3.10. U.S. Environmental Protection Agency (2001).

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Type: Other, see. remarks
Light Source:
Light spect.:
Rel. intensity: Based on intensity of sunlight
Degradation: 37 hour half-life
Method:
GLP:
Test substance: butanol
Remark: Atmospheric photo-oxidation potential was estimated using the submodel AOPWIN that calculates a second order half-life with units of cm^3/molecules-cm. Vapor phase butanol is expected to degrade in the atmosphere by reaction with photochemically produced hydroxyl (OR) radicals. Chemical-specific input parameters for EPIWIN modeling were: molecular weight 74.12 g/mol, vapor pressure 0.42 mm Hg, log Kow 0.88, melting point -89.9°C, boiling point 117.6°C and aqueous solubility 77,000 mg/L. The second order rate constant was calculated as 6.89 E-12 cm3/(molecule-sec) at 25°C.
Based on 1.56E6 OH molecules/cm3 and assuming 12 hours of sunlight per day, the estimated half-life was 1.552 days or 37 hours.
Reliability: (2) valid with restrictions, calculated value
References: Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere. 26: 2293-2299.

Meylan, W. and PH Howard. 2000a. User's Guide for AOPWIN, Version 1.90. EPIWIN (Estimation Program Interface for Windows) version 3.10. U.S. Environmental Protection Agency, 2000.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Method: other (measured): method not stated
Year: 1994
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: Measured rate constant: 12.5E-12 cm^3/molecule.sec
Half-life: 30.8 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm^3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).

Reliability: (2) valid with restrictions
Value obtained from a recognised source of atmospheric degradation data.
Flag: Critical study for SIDS endpoint
Reference: Kwok, E.S.C. and Atkinson, R., 1994 (from SRC AOPWIN v1.91 Experimental Database).
15-SEP-2005 (33)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Method: other (measured): method not stated
Year: 1994
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Result: Measured rate constant: 14.4 x 10^{-12} cm^3/molecule.sec
Half-life: 26.7 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).
Reliability: (2) valid with restrictions
Value obtained from a recognised source of atmospheric degradation data.
Flag: Critical study for SIDS endpoint
Reference: Atkinson, R., 1994 (from SRC AOPWIN v1.91 Experimental Database).
29-DEC-2005 (11)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Remark: The photooxidation half-life in air for the gas-phase reaction with hydroxyl radicals was 0.24-2.4 hours, based on the rate of disappearance of hydrocarbon. The measured rate constant of 1.195x10^{-11} cm3/molecule*sec for the vapor-phase reaction with photochemically produced hydroxyl radicals of 5x10^5/cm^3 at 25 degree C in air corresponds to an atmospheric half-life of 1.3 days.
Reliability: (2) valid with restrictions
Reference: Atkinson, R. 1987a. Estimation of OH radical rate constants and atmospheric lifetimes for polychlorobiphenyls, dibenzo-p-dioxins. Environ. Sci. Technol. 21: 305-307.

Darnall, K.R., Lloyd, A.C., Winer, A.M., and Pitts, Jr., J.N. 1976. Reactivity scale for the atmospheric

hydrocarbons based on reaction with hydroxyl radical.
Environ. Sci. Technol. 10(7): 692-696.
29-DEC-2005 (9) (36)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Test substance: > 90% 1-octanol (111-87-5)

Remark: The rate constant for the vapor-phase reaction of octanol with photochemically produced hydroxyl radicals in air has been estimated to be 1.195×10^{-11} cm^3/molecule*sec at 25 degree C, which corresponds to an atmospheric half-life of about 1.3 days at an atmospheric concentration of 5×10^5 hydroxyl radicals/cm^3.
Test substance: Octanol (111-87-5)
Reliability: (4) not assignable
Textbook used for background information.
Reference: Atkinson, R. 1987b. Intern. J. Chem. Kin. 19:799-828. (cited in HSDB).

Lyman, W.J., Reehl, W.F., and Rosenblatt, D.H. 1982. Handbook on Chemical Property Estimation Methods, Environmental Behaviour of Organic Compounds. New York: McGraw-Hill.

Silverstien, R.M. and Bassler, G.C. 1963. Spectometric Id. Org. Cmpd. New York: J. Wiley & Sons Inc. (cited in HSDB).
29-DEC-2005 (10) (79) (107)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Method: other (calculated): SRC AOPWIN v1.91
Year: 2004
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Method: The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
Result: Estimated rate constant: 15.36831E-12 cm3/molecule.sec
Half-life: 25.1 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).
Reliability: (2) valid with restrictions
This result was estimated using a standard calculation method,

validated by limited measured data.
Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.
21-DEC-2005 (4)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Method: other (calculated): SRC AOPWIN v1.91
Year: 2006
GLP: no
Test substance: 1-dodecanol (112-53-8)

Method: The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
Result: Estimated rate constant: 18.1944E-12 cm3/molecule.sec
Half-life: 7.054 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).
Reliability: (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
Reference: SRC AOPWIN v1.91. US EPA, 2006.
04-APR-07

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Method: other (calculated): SRC AOPWIN v1.91
Year: 2004
GLP: no
Test substance: 1-tetradecanol (112-72-1)

Method: The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
Result: Estimated rate constant: 21.02050E-12 cm3/molecule.sec
Half-life: 18.3 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).
Reliability: (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.

Flag: Critical study for SIDS endpoint
Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.
21-DEC-2005 (5)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: other: UV lamp

Method: other (measured): microphotoreactor developed by Lotz et al, modified by Kotzias et al.
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: Exposure period: 17 hours
Temperature: 15 degrees C
Test concentration: 1680 ng/g Silica gel
UV lamp at 290 nm
Result: 3.1% mineralisation (CO2), and 0.5% (organic fragments)
Reliability: (4) not assignable
Documentation insufficient for assessment. A source of higher reliability is available.
Reference: Freitag, D. et al., Ecotoxicol. Environ. Saf. 6, 60-81 (1982).
09-JAN-2005 (26)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Method: other (calculated): SRC AOPWIN v1.91
Year: 2004
GLP: no
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
Result: Estimated rate constant: 23.84660E-12 cm3/molecule.sec
Half-life: 16.2 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).
Reliability: (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
Reference: Annex V (2005). Environmental Fate Data: QSAR predictions

and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.
21-DEC-2005 (5)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Method: other (calculated): SRC AOPWIN v1.91
Year: 2006
GLP: no
Test substance: octadecanol (112-92-5)

Method: The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
Result: Estimated rate constant: 26.53271E-12 cm3/molecule.sec
Half-life: 4.812 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).
Reliability: (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
Reference: SRC AOPWIN v1.91. US EPA, 2006.
04-APR-07

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Method: other (calculated): SRC AOPWIN v1.91
Year: 2004
GLP: no
Test substance: 1-eicosanol (629-96-9)

Method: The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
Result: Estimated rate constant: 29.49879E-12 cm3/molecule.sec
Half-life: 13.1 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).

Branched components may be photodegraded slightly faster than linear components of equivalent carbon number, but the reported half-life represents a reasonably conservative estimate for this substance.

Reliability: (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.
21-DEC-2005 (3)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Method: other (calculated): SRC AOPWIN v1.91
Year: 2004
GLP: no
Test substance: 1-docosanol (661-19-8)

Method: The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
Result: Estimated rate constant: 32.32488E-12 cm3/molecule.sec
Half-life: 11.9 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).
Reliability: (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
Flag: Critical study for SIDS endpoint
Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.
21-DEC-2005 (3)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Method: other (calculated): SRC AOPWIN v1.91
Year: 2006
GLP: no
Test substance: 1-tetracosanol (506-51-4)

Method: The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
Result: Estimated rate constant: 35.1510E-12 cm3/molecule.sec
Half-life: 3.651 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3

(global average value, obtained from EU Technical Guidance for environmental risk assessment).

Reliability: (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.

Reference: SRC AOPWIN v1.91. US EPA, 2006.

04-APR-07

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Method: other (calculated): SRC AOPWIN v1.91
Year: 2006
GLP: no
Test substance: 1-hexacosanol (506-52-5)

Method: The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.

Result: Estimated rate constant: 37.9771E-12 cm3/molecule.sec
Half-life: 3.380 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).

Reliability: (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.

Reference: SRC AOPWIN v1.91. US EPA, 2006.

04-APR-07

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Method: other (calculated): SRC AOPWIN v1.91
Year: 2006
GLP: no
Test substance: 1-octacosanol (557-61-9)

Method: The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.

Result: Estimated rate constant: 40.8032E-12 cm3/molecule.sec
Half-life: 3.146 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).

Reliability: (2) valid with restrictions

This result was estimated using a standard calculation method, validated by limited measured data.
04-APR-07

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Method: other (calculated): SRC AOPWIN v1.91
Year: 2006
GLP: no
Test substance: 1-triacontanol (593-50-0)

Method: The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
Result: Estimated rate constant: 43.6293E-12 cm3/molecule.sec
Half-life: 2.942 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3 (global average value, obtained from EU Technical Guidance for environmental risk assessment).
Reliability: (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
Reference: SRC AOPWIN v1.91. US EPA, 2006.
04-APR-07

3.1.2 Stability in Water

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Abiotic
Method	other (calculated)
Year	1990
GLP	no data
Test substance	other TS: 100% ethanol
Remark	Duration (days) of test: Not relevant. Positive/negative controls: Not relevant. Analytical procedures used to measure test substance loss: Not relevant. Reference is to method. According to Lyman et al. both alkanes and alcohols are resistant to hydrolysis.
Result	Ethanol is not expected to undergo hydrolysis. (This is deduced from basics according to Lyman et al. (1990)).
Reliability	(2) valid with restrictions

Reference Lyman, W., Reehl, W., Rosenblatt, D. (1990) Handbook of Chemical Property Estimation Methods: Environmental Behaviour of Organic Compounds. American Chemical Society, Washington, DC.

19.10.2004 (55)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type Abiotic
t1/2 pH4
t1/2 pH7 = 2 year
t1/2 pH9
Deg. product
Method other
Year
GLP no data
Test substance ethanol (64-17-5)

Remark Ethanol is stable in water and is not hydrolysed. Hydrolysis as a function of pH is, therefore, an irrelevant endpoint.
Half-life calculated from the rate constant for the reaction with hydroxyl radicals (1.1×10^9) at room temperature (15 - 25°C). Actual figure for half-life given in ENVIROFATE database (Environmental Fate. SilverPlatter, Chem-Bank, June1993).

Result Half-lives of between 334 days and 36.6 years have been calculated for photooxidation in water based on the same rate constant (Handbook of Environmental Degradation Rates (1991) Eds Howard, P.H. et al. Lewis Publishers, Michigan).
Reliability (2) valid with restrictions
Reference Anbar, M. & Neta, P. (1967) A compilation of specific bimolecular rate constants for the reactions of hydrated electrons, hydrogen atoms and hydroxyl radicals with inorganic and organic compounds in aqueous solution. Int. J. Appl. Radiation & Isotopes 18, 493 - 523.
(56)

19.10.2004

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Type: Volatilization from surface waters
Test substance: 1-butanol

Method: Calculated using EPISUITE v3.10 (U.S. EPA, 2001)
Result: Half-life from model river: 39.51 days
Half-life from model lake: 434.1 days
Remark: Based on Henry's law constant of 5.3 E-7 atm-m3/mol, vapor pressure of 0.42 mm Hg, water solubility of 77 ,000 mg/L, and a molecular weight of 74.12

g/mole, and model defaults (for model river: river 1 m deep, water flow at 1 m/sec, wind speed of 5 m/sec; for model lake: 1 m deep, water flow 0.05 m/sec, wind speed 0.5 m/sec).
GLP: Not applicable .
Reliability: (2) valid with restrictions, calculated values
Reference: EPISUITE v. 3.10, U.S. Environmental Protection Agency, April 2001.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Test substance: >95% 1-hexanol (111-27-3)

Remark: This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
Reference: IUCLID Data Set: 1-Hexanol. Shell Chemicals Ltd. May 11, 2006.
10-JAN-2005

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: abiotic

GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Remark: Photolysis or hydrolysis of octanol in aquatic systems is not expected to be important.
Reliability: (4) not assignable
Textbook used for background information.
Flag: Critical study for SIDS endpoint
Reference: Lyman, W.J., Reehl, W.F., and Rosenblatt, D.H. 1982. Handbook on Chemical Property Estimation Methods, Environmental Behaviour of Organic Compounds. New York: McGraw-Hill.

U.S. Environmental Protection Agency (USEPA). 1987. EXAMS II Computer Simulation.
10-JAN-2005 (79) (114)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Test substance: > 90% 1-octanol (111-87-5)

Remark: Alcohols are generally resistant to hydrolysis. Alcohols absorb UV light at wavelengths <185 nm, which is not in the environmentally significant range of >290 nm. Likewise, alcohols are commonly used as solvents for obtaining UV

spectra. Therefore octanol probably will not undergo hydrolysis or direct photolysis in the environment.

Source: Atkinson, R. 1987b. Intern. J. Chem. Kin. 19:799-828. (cited in HSDB)

Test substance: Octanol (111-87-5)

Reliability: (4) not assignable
Textbook used for background information.

References: Atkinson, R. 1987b. Intern. J. Chem. Kin. 19:799-828. (cited in HSDB)

Lyman, W.J., Reehl, W.F., and Rosenblatt, D.H. 1982. Handbook on Chemical Property Estimation Methods, Environmental Behaviour of Organic Compounds. New York: McGraw-Hill.

Silverstien, R.M. and Bassler, G.C. 1963. Spectometric Id. Org. Cmpd. New York: J. Wiley & Sons Inc. (cited in HSDB)

11-OCT-2005 (10) (79) (107)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Test substance: 1-decanol (112-30-1)

Remark: This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.

Flag: Critical study for SIDS endpoint

Reference: IUCLID Data Set: 1-Decanol. Shell Chemicals Ltd. May 11, 2006.

09-SEP-2005

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type: Volatilization from surface waters

Test substance: 1-dodecanol

Method: Calculated using EPISUITE v3.12 (U.S. EPA, 2006)

Result: Half-life from model river: 1.558 days
Half-life from model lake: 21.77 days

Remark: Based on Henry's law constant of 2.22 E-5 atm-m3/mol and a molecular weight of 186.34 g/mole, and model defaults (for model river: river 1 m deep, water flow at 1 m/sec, wind speed of 5 m/sec; for model lake: 1 m deep, water flow 0.05 m/sec, wind speed 0.5 m/sec).

GLP: Not applicable .

Reliability: (2) valid with restrictions, calculated values

Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Remark: This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
Flag: Critical study for SIDS endpoint
Reference: IUCLID Data Set: 1-Tetradecanol. Shell Chemicals Ltd. May 11, 2006.
10-JAN-2005

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Test substance: 1-hexadecanol (36653-82-4)

Remark: This substance has no hydrolysable structural features and would be expected to be stable in respect of hydrolysis. Oxidation would not be expected under normal environmental conditions.
Flag: Critical study for SIDS endpoint
Reference: IUCLID Data Set: 1-Hexadecanol. Shell Chemicals Ltd. May 11, 2006.
09-JAN-2005

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Type: Volatilization from surface waters
Test substance: 1-octadecanol

Method: Calculated using EPISUITE v3.12 (U.S. EPA, 2006)
Result: Half-life from model river: 0.1176 days
Half-life from model lake: 7.029 days
Remark: Based on Henry's law constant of 8.41 E-4 atm-m3/mol and a molecular weight of 270.50 g/mole, and model defaults (for model river: river 1 m deep, water flow at 1 m/sec, wind speed of 5 m/sec; for model lake: 1 m deep, water flow 0.05 m/sec, wind speed 0.5 m/sec).

GLP: Not applicable .
Reliability: (2) valid with restrictions, calculated values
Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Test substance: 1-eicosanol (629-96-9)

Remark: This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
Flag: Critical study for SIDS endpoint

Reference: IUCLID Data Set: Icosan-1-ol. Shell Chemicals Ltd. May 11, 2006.
10-JAN-2005

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Remark: This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
Flag: Critical study for SIDS endpoint
Reference: IUCLID Data Set: Docosan-1-ol. Shell Chemicals Ltd. May 11, 2006.
09-JAN-2005

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Type: Volatilization from surface waters
Test substance: 1-tetracosanol

Method: Calculated using EPISUITE v3.12 (U.S. EPA, 2006)
Result: Half-life from model river: 0.09597 days
Half-life from model lake: 7.627 days
Remark: Based on Henry's law constant of 2.89 E-3 atm-m3/mol and a molecular weight of 354.67 g/mole, and model defaults (for model river: river 1 m deep, water flow at 1 m/sec, wind speed of 5 m/sec; for model lake: 1 m deep, water flow 0.05 m/sec, wind speed 0.5 m/sec).

GLP: Not applicable .
Reliability: (2) valid with restrictions, calculated values
Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Type: Volatilization from surface waters
Test substance: 1-hexacosanol

Method: Calculated using EPISUITE v3.12 (U.S. EPA, 2006)
Result: Half-life from model river: 0.09256 days
Half-life from model lake: 7.845 days
Remark: Based on Henry's law constant of 5.09 E-3 atm-m3/mol and a molecular weight of 382.72 g/mole, and model defaults (for model river: river 1 m deep, water flow at 1 m/sec, wind speed of 5 m/sec; for model lake: 1 m deep, water flow 0.05 m/sec, wind speed 0.5 m/sec).

GLP: Not applicable .
Reliability: (2) valid with restrictions, calculated values
Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Type:	Volatilization from surface waters
Test substance:	1-octacosanol
Method:	Calculated using EPISUITE v3.12 (U.S. EPA, 2006)
Result:	Half-life from model river: 0.09169 days Half-life from model lake: 8.081 days
Remark:	Based on Henry's law constant of 8.97 E-3 atm-m3/mol and a molecular weight of 410.77 g/mole, and model defaults (for model river: river 1 m deep, water flow at 1 m/sec, wind speed of 5 m/sec; for model lake: 1 m deep, water flow 0.05 m/sec, wind speed 0.5 m/sec).
GLP:	Not applicable .
Reliability:	(2) valid with restrictions, calculated values
Reference:	EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Type:	Volatilization from surface waters
Test substance:	1-triacontanol
Method:	Calculated using EPISUITE v3.12 (U.S. EPA, 2006)
Result:	Half-life from model river: 0.0923 days Half-life from model lake: 8.326 days
Remark:	Based on Henry's law constant of 1.58 E-2 atm-m3/mol and a molecular weight of 438.83 g/mole, and model defaults (for model river: river 1 m deep, water flow at 1 m/sec, wind speed of 5 m/sec; for model lake: 1 m deep, water flow 0.05 m/sec, wind speed 0.5 m/sec).
GLP:	Not applicable .
Reliability:	(2) valid with restrictions, calculated values
Reference:	EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.

3.3.1 Distribution (%)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Media	air - biota - sediment(s) - soil - water
Method	Calculation according Mackay, level III
Year	2001
Test substance	ethanol (64-17-5)
Remark	Adsorption coefficient: Not given. Desorption: Not given. Volatility: Not given.

	Model used: EQC model of Mackay et al. (1996). Version 1.01 Date: 1997. The following input parameters were used: MWt 46.09 g/mol Temp. 25 deg C Water solubility 716,000 g/m^3 calculated from vapour pressure and Henry's law constant of 5e-06 atm.m^3/mol (Gaffney, 1987) Vapour Pressure 7870 Pa (59.03 mm Hg) log Kow -0.31 Melting point –114 deg. C t1/2 air 203 hr (Graedel, 1978) t1/2 water 182 hr (from biodegradation data) t1/2 sediment 210 hr (from biodegradation data) Environmental conditions: left at the default values of the model.
Result	Air 13.0% 1.60e-8 mol/m^3 (738 ng/m^3) Water 44.8% 2.75e-5 mol/m^3 (1271 ng/l) Soil 42.1 % 2.88e-4 mol/m^3 (8.3 ng/g) Sediment 0.039% 9.50e-6 mol/m^3 (0.34 ng/g) Adsorption coefficient, desorption and volatility not given. At steady state 67% of additional inputs of ethanol are lost through reactions and 33% are lost through advection.
Reliability	(2) valid with restrictions
Reference	Mackay, D. DiGuardo, A, Paterson, S. and Cowan, C. (1996) Evaluating the environmental fate of a variety of types of chemicals using the EQC model. Env. Toxicol. Chem. 15 (9): 1627-1637. See http://www.trentu.ca/academic/aminss/envmodel/EQCD.html
19.10.2004	(65) (66)

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Type:	Level III Fugacity-based distribution modeling
Test substance:	1-butanol (CAS No. 71-36-3)
Method:	Level III fugacity based model, EPISUITE v. 3.10
GLP:	Not applicable
Remark:	Default values were assumed for environmental compartment descriptions, dimensions, and properties, advective and dispersive properties. Chemical-specific parameters were: molecular weight (74.12 g/mol), vapor pressure (0.56 hPa or 0.42 mm Hg), log Kow (0.88), melting point -89.9°C, aqueous solubility 77,000 mg/L, boiling point of 117.6°C, and a Henry's Law

constant of 5.3 E-7 atm-m3/mol. Half-lives calculated by the model based on the properties of the test substance were: water and soil half-lives 208 hr, and sediment half-life 832 hr. half-life in air was 30 hours and was based on a second-order rate constant for atmospheric hydroxy radical-mediated photooxidation of 8.57 E-12 cm3/molecule-sec that was cited in EPISUITE (Kwok E, Atkinson R, 1994). No other information on the measured value was available, but was used by the model based on a 12 hour day and assuming 15 E+6 HO molecules/cm3. Physical properties were the preferred values from the SIDS dossier.

Emissions were assumed to be only to air. Due to its uses as a solvent and manufacture with closed systems, essentially all releases will be through its uses. Releases to soil and water will be negligible, compared to air releases.

Distribution: Air (40.2%), Water (15;7%), Soil (44.1 %), Sediment (>0.1 %)
Source: EPISUITE v. 3.10, U.S. Environmental Protection Agency, April 2001.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Method: other: Mackay Level I and Level III models
Year: 2005

Result: INPUT DATA USED:
Molecular weight 102.2
Data temperature 25 deg C
Log Kow 2.03
Water Solubility 5900 mg/l
Vapour pressure 122 Pa
Melting point -50 deg C
Half-life in air 30.8 h
Half-life in water and soil 720 h
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:
Air 28%
Soil 6.23%
Water 65.6%
Fish 3.52E-04%
Sediment 0.14%

The Level III program has also been used, with the default model, using the same input parameters.The distribution between compartments obtained is as follows:

Release:	To air	To water	To soil
% in air	66.8	0.0375	0.0379

% in water 8.11 99.9 14.6
% in sediment 0.00728 0.0897 0.0131
% in soil 25.1 0.0141 85.3
The results reflect that the ultimate fate of 1-hexanol is dependent on its route of release into the environment.

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and principles.

Flag: Critical study for SIDS endpoint

Reference: Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.
21-DEC-2005 (4)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Method: other: Mackay Level I and Level III models
Year: 2005

Remark: An evaporation rate of 1.75x10-6 mol/cm^2*h was determined by gravimetric method with an air flow rate of 50 L/h at 20 degree C. Based on calculated Henry's law constant, half-life from a model river of 1 meter deep flowing at 1 m/sec with a wind speed of 3 m/sec has been estimated to be 1.8 days. The half-life from a model pond with the consideration of adsorption, has been estimated to be about 82 days.

Result: INPUT DATA USED:
Molecular weight 130.2
Data temperature 25 deg C
Log Kow 3.15
Water Solubility 551 mg/l
Vapour pressure 10 Pa
Melting point -16 deg C
Half-life in air 26.7 h
Half-life in water and soil 720 h

RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:
Air 17.3%
Soil 45.4%
Water 36.3%
Fish 2.56E-03%
Sediment 1.01%

The Level III program has also been used, with the default model, using the same input parameters.

The distribution between compartments obtained is as follows:

Release:	To air	To water	To soil
% in air	63.6	0.0407	0.00446
% in water	4.02	98.7	1.6
% in sediment	0.0504	1.24	0.02
% in soil	32.3	0.0207	98.4

The results reflect that the ultimate fate of 1-octanol is dependent on its route of release into the environment. 1-Octanol released to air would partially precipitate to soil.There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility.

Test substance: 1-octanol (111-87-5)

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and principles.

Flag: Critical study for SIDS endpoint

Reference: Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

21-DEC-2005 (6)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Method: other: Mackay Level I and Level III models

Year: 2005

Result: INPUT DATA USED:
Molecular weight 158.3
Data temperature 25 deg C
Log Kow 4.57
Water Solubility 39.5 mg/l
Vapour pressure 1.13 Pa
Melting point 6.4 deg C
Half-life in air 25.1 h
Half-life in water and soil 720 h

RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

Air 2.57%
Soil 92.5%
Water 2.81%
Fish 5.22E-03%
Sediment 2.06%

The Level III program has also been used, with the default model, using the same input parameters.
The distribution between compartments obtained is as follows:

Release:	To air	To water	To soil
% in air	71.9	0.0324	0.000287
% in water	3.18	45.9	0.0674
% in sediment	3.74	54	0.0792
% in soil	21.2	0.00954	9.9

The results reflect that the ultimate fate of 1-decanol is dependent on its route of release into the environment.
1-Decanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility. In water, the adsorption coefficient of 1-decanol results in significant adsorption to sediment.

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and principles.

Flag: Critical study for SIDS endpoint

Reference: Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

21-DEC-2005 (5)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)</u>

Method: other: Mackay Level III model

Year: 2006

Result: INPUT DATA USED:
Molecular weight 186.34
Data temperature 25 deg C
Log Kow 5.13
Vapour pressure 0.00181 mm Hg
Liquid VP 0.00199 mm Hg
Melting point 29.2 deg C
Soil Koc 5.53 x 10^4
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level III model is as follows:

Release:	Mass Amount (%)
% in air	0.989
% in water	16.3

% in sediment 58.2
% in soil 24.5

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and principles.
Flag: Critical study for SIDS endpoint
Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.
04-APR-2007

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Method: other: Mackay Level I and Level III models
Year: 2005

Result: INPUT DATA USED:
Molecular weight 214.4
Data temperature 25 deg C
Log Kow 6.03
Water Solubility 0.191 mg/l
Vapour pressure 0.014 Pa
Melting point 40 deg C
Half-life in air 18.3 h
Half-life in water and soil 720 h
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

Air 0.33%
Soil 97.3%
Water 0.10%
Fish 5.50E-03%
Sediment 2.16%
The Level III program has also been used, with the default model, using the same input parameters.The distribution between compartments obtained is as follows:

Release:	To air	To water	To soil
% in air	38.4	0.00395	0.000033
% in water	1.57	4.61	0.0106
% in sediment	32.5	95.4	0.219
% in soil	27.6	0.00284	99.8

The results reflect that the ultimate fate of 1-tetradecanol is dependent on its route of release into the environment. 1-Tetradecanol released to air would partially precipitate to

soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility. In water, the adsorption coefficient of 1-tetradecanol results in significant adsorption to sediment.

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and

Flag: Critical study for SIDS endpoint

Reference: Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

21-DEC-2005 (6)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Method: other: Mackay Level I and Level III models

Year: 2005

Result: INPUT DATA USED:
Molecular weight 242.4
Data temperature 25 deg C
Log Kow 6.65
Water Solubility 0.013 mg/l
Vapour pressure 0.0014 Pa
Melting point 50 deg C
Half-life in air 16.2 h
Half-life in water and soil 720 h

RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

Air	0.13%
Soil	97.6%
Water	0.03%
Fish	5.51E-03%
Sediment	2.17%

The Level III program has also been used, with the default model, using the same input parameters. The distribution between compartments obtained is as follows:

Release:	To air	To water	To soil
% in air	9.88	0.00125	1.34E-05
% in water	1.25	2.98	0.0103
% in sediment	40.7	97	0.335
% in soil	48.2	0.00609	99.7

The results reflect that the ultimate fate of 1-hexadecanol is

dependent on its route of release into the environment. 1-Hexadecanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility. In water, the adsorption coefficient of 1-hexadecanol results in significant adsorption to sediment.

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and principles.

Flag: Critical study for SIDS endpoint

Reference: Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

21-DEC-2005 (6)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Method: other: Mackay Level III model

Year: 2006

Result: INPUT DATA USED:
Molecular weight 270.5
Data temperature 25 deg C
Log Kow 7.72
Vapour pressure 1.83 x 10^{-6} mm Hg
Liquid VP 7.48 x 10^{-6} mm Hg
Melting point 86.8 deg C
Soil Koc 2.15 x 10^{7}
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level III model is as follows:

Release:	Mass Amount (%)
% in air	0.317
% in water	3.79
% in sediment	28.8
% in soil	67.1

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and principles.

Flag: Critical study for SIDS endpoint

Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.

04-APR-2007

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Method: other: Mackay Level I and Level III models
Year: 2005

Result: INPUT DATA USED:
Molecular weight 298.5
Data temperature 25 deg C
Log Kow 7.75
Water Solubility 0.0011 mg/l
Vapour pressure 0.000015 Pa
Melting point 66 deg C
Half-life in air 13.1 h
half-life in water and soil 720 h
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:
Air 1.61E-03%
Soil 97.8%
Water 1.96E-03%
Fish 5.52E-03%
Sediment 2.17%

The Level III program has also been used, with the default model, using the same input parameters.The distribution between compartments obtained is as follows:

Release:	To air	To water	To soil
% in air	0.639	2.52E-05	2.41E-07
% in water	1.22	2.5	0.0111
% in sediment	47.5	97.5	0.433
% in soil	50.6	0.00199	99.6

The results reflect that the ultimate fate of 1-eicosanol is dependent on its route of release into the environment. 1-Eicosanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility. In water, the adsorption coefficient of 1-eicosanol results in significant adsorption to sediment.
Reliability: (2) valid with restrictions
Assessment performed according to accepted models and
Flag: Critical study for SIDS endpoint
Reference: Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.
21-DEC-2005 (4)

<u>1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)</u>

Method: other: Mackay Level I and Level III models
Year: 2005

Result: INPUT DATA USED:
Molecular weight 326.6
Data temperature 25 deg C
Log Kow 7.75
Water Solubility 0.001 mg/l
Vapour pressure 0.00000815 Pa
Melting point 72.5 deg C
half life in air 11.9 h
half life in water and soil 720 h

RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:
Air 1.05E-03%
Soil 97.8%
Water 1.96E-03%
Fish 5.52E-03%
Sediment 2.17%

The Level III program has also been used, with the default model, using the same input parameters. The distribution between compartments obtained is as follows:

Release:	To air	To water	To soil
% in air	0.582	1.72E-05	1.71E-07
% in water	1.22	2.5	0.0111
% in sediment	47.5	97.5	0.434
% in soil	50.7	0.00149	99.6

The results reflect that the ultimate fate of 1-docosanol is dependent on its route of release into the environment. 1-Docosanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility. In water, the adsorption coefficient of 1-docosanol results in significant adsorption to sediment.

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and principles,

Flag: Critical study for SIDS endpoint

Reference: Annex VI (2005). Environmental Distribution Modelling;

Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.
21-DEC-2005 (4)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Method: other: Mackay Level III model
Year: 2006

Result: INPUT DATA USED:
Molecular weight 354.67
Data temperature 25 deg C
Log Kow 10.7
Vapour pressure 2.4 x 10^{-9} mm Hg
Liquid VP 3.37 x 10^{-8} mm Hg
Melting point 141 deg C
Soil Koc 1.87 x 10^{10}
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level III model is as follows:

Release:	Mass Amount (%)
% in air	0.188
% in water	3.57
% in sediment	31.2
% in soil	65.1

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and principles.
Flag: Critical study for SIDS endpoint
Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.
04-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Method: other: Mackay Level III model
Year: 2006

Result: INPUT DATA USED:
Molecular weight 382.72
Data temperature 25 deg C
Log Kow 11.7
Vapour pressure 2.16 x 10^{-9} mm Hg
Liquid VP 4.57 x 10^{-8} mm Hg
Melting point 159 deg C
Soil Koc 1.83 x 10^{11}

RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level III model is as follows:

Release:	Mass Amount (%)
% in air	0.179
% in water	3.58
% in sediment	31
% in soil	65.3

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and principles.
Flag: Critical study for SIDS endpoint
Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.
04-APR-2007

<u>1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)</u>

Method: other: Mackay Level III model
Year: 2006

Result: INPUT DATA USED:
Molecular weight 410.77
Data temperature 25 deg C
Log Kow 12.6
Vapour pressure 4.02 x 10^{-10} mm Hg
Liquid VP 1.28 x 10^{-8} mm Hg
Melting point 177 deg C
Soil Koc 1.75 x 10^{12}
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level III model is as follows:

Release:	Mass Amount (%)
% in air	0.0676
% in water	1.82
% in sediment	30.9
% in soil	67.2

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and principles.
Flag: Critical study for SIDS endpoint
Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.
04-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Method: other: Mackay Level III model
Year: 2006

Result: INPUT DATA USED:
Molecular weight 438.83
Data temperature 25 deg C
Log Kow 13.6
Vapour pressure 7.1 x 10^{-11} mm Hg
Liquid VP 2.93 x 10^{-9} mm Hg
Melting point 188 deg C
Soil Koc 1.67 x 10^{13}
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level III model is as follows:

Release:	Mass Amount (%)
% in air	0.0643
% in water	1.83
% in sediment	30.8
% in soil	67.3

Reliability: (2) valid with restrictions
Assessment performed according to accepted models and principles.
Flag: Critical study for SIDS endpoint
Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.
04-APR-2007

3.3.2 Stability in Soil (Koc)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Media Other
Method
Year
Test substance ethanol (64-17-5)
Remark PCKOCWIN v1.66 Results

First Order Molecular Connectivity Index .....: 1.414 Non-Corrected Log Koc .....: 1.3755 Fragment Correction(s):
1 Aliphatic Alcohol (-C-OH) .....: -1.5193

Corrected Log Koc .....: -0.1438
Over Correction Adjustment to Lower Limit Log Koc: 0.0000

Estimated Koc: 1

Reference U.S. EPA URL http://www.epa.gov/opptintr/exposure/docs/episuite.htm
19.10.2004 (64)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Type: Soil or sediment partition coefficient (Koc)
Test substance: 1-butanol (CAS No. 71-36-3)
Method: Calculated using EPISUITE v. 3.10 and PCKOCWIN v. 1.66 using structural features of the molecule
Result: 2.44 L/kg
GLP: not applicable
Reliability: (2) valid with restrictions, calculated values
Reference: EPISUITE v. 3.10, U.S. Environmental Protection Agency, April 2001.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Media: water - soil
Method: other (calculation): various methods

Method: Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance.

The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 2.03 was used in the TGD calculation methods.

Result: TGD Hydrophobics method: Koc = 56
TGD Hydrophobics method: Koc = 118
TGD Alcohols method: Koc = 19.6
SRC PCKOCWIN method: Koc = 8.3
Test substance: 1-hexanol (111-27-3)
Reliability: (2) valid with restrictions
The value was predicted using accepted calculation methods
Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long

Chain Aliphatic Alcohols Category SIAR.
28-DEC-2005 (3)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Media: water - soil
Method: other (calculation): various methods
Year: 2004

Method: Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances. The measured log Kow value of 3.15 was used in the TGD calculation methods.
Result: TGD Hydrophobics method: Koc = 448
TGD Non-hydrophobics method: Koc = 455.0
TGD Alcohols method: Koc = 53.5
SRC PCKOCWIN method: Koc = 28.3
Test Substance: 1-octanol (111-87-5)
Reliability: (2) valid with restrictions
The value was predicted using accepted calculation methods.
Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.
28-DEC-2005 (5)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Media: water - soil
Method: other (calculation): various methods
Year: 2004

Method: Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 4.57 was used in the TGD calculation methods.

Result: TGD Hydrophobics method: Koc = 6330
TGD Non-hydrophobics method: Koc = 2490
TGD Alcohols method: Koc = 190
SRC PCKOCWIN method: Koc = 96

Test substance: 1-decanol (112-30-1)

Reliability: (2) valid with restrictions
The value was predicted using accepted calculation methods.

Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

28-DEC-2005 (4)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)</u>

Type: Soil or sediment partition coefficient (Koc)
Test substance: 1-dodecanol
Method: Calculated using EPISUITE v. 3.12 and PCKOCWIN v. 1.66 using structural features of the molecule
Result: 327.1
GLP: not applicable
Reliability: (2) valid with restrictions, calculated values
Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)</u>

Method: Measurement of the sorption of five alcohols onto a mixture of activated sludge and river water suspended solids. River water was collected from River Gowy, Ellesmere Port, on two successive days and mixed then sterilised. It contained 12 mg/L suspended solids. Activated sludge was obtained from a municipal waste water treatment plant. The mixed liquor suspended solids content was determined to be 2940 mg/L. Total organic carbon was 880 mg/L. The mixture was sterilised, allowed to settle, and a simulated effluent was prepared to give 30 mg/L suspended solids. The fraction of organic carbon was 0.167. The vessel was spiked with TS to give ca. 100 µg/L. The test system was stirred for 24 h, which was sufficient to give equilibrium. The mixed settled activated sludge with river water with up to 72 h equilibration.

Remark: The results for five substances are considered alongside each other since the results of the whole study are useful for comparison purposes. The data for the alcohol ethoxylates obtained in the study do not need to be included in this summary.

Result: Alcohol sorption coefficients showed some time dependence, reaching a plateau by 72 h. C15 was found to be an unexplained outlier. The 72 h results were:

C	12	14	15	16	18
Kd	3000± 80	8490± 920	3080± 270	23800 ±3200	78700 ±5400
Koc	17980	50830	-	143000	471000
log Koc	4.25	4.71	-	5.15	5.67

These data (neglecting the C15) can be interpreted as a QSAR in the usual way as:

Log Koc = 0.11 + 0.77 log Kow

R2 = 0.994

The result is in line with typical QSARs of this type.

Test substance: > 95% 1-Tetradecanol (112-72-1); Linear alcohols labelled with 14-C, radiochemical purity 99%.

Reliability: (2) valid with restrictions
Although not a SIDS end point, this study is considered to be the best study of Koc for these carbon numbers.

Reference: R. van Compernolle, D. McAvoy, A. Sherren, T. Wind, M.L. Cano, S.E. Belanger, P.B. Dorn, K.M. Kerr, "Predicting the sorption of fatty alcohols and alcohol ethoxylates to effluent and receiving water". Ecotox. and Environ. Safety, in press.

21-DEC-2005 (55)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Method: other (calculation): various methods
Year: 2004

Method: Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.
The measured log Kow value of 6.03 was used in the TGD calculation methods.

Result: TGD hydrophobics method: Koc = 96500

TGD Non-hydrophobics method: Koc = 14300
TGD Alcohols method: Koc = 710
SRC PCKOCWIN method: Koc = 1110

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

Test substance: 1-tetradecanol (112-72-1)

Reliability: (2) valid with restrictions
The value was predicted using accepted calculation methods.

Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

28-DEC-2005 (5)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)</u>

Method: Measurement of the sorption of five alcohols onto a mixture of activated sludge and river water suspended solids.
River water was collected from River Gowy, Ellesmere Port, on two successive days and mixed then sterilised. It contained 12 mg/L suspended solids.

Activated sludge was obtained from a municipal waste water treatment plant. The mixed liquor suspended solids content was determined to be 2940 mg/L. Total organic carbon was 880 mg/L. The mixture was sterilised, allowed to settle, and a simulated effluent was prepared to give 30 mg/L suspended solids. The fraction of organic carbon was 0.167. The vessel was spiked with TS to give ca. 100 µg/L. The test system was stirred for 24 h, which was sufficient to give equilibrium.

The mixed settled activated sludge with river water with up to 72 h equilibration.

Remark: The results for five substances are considered alongside each other since the results of the whole study are useful for comparison purposes.
The data for the alcohol ethoxylates obtained in the study do not need to be included in this summary.

Result: Alcohol sorption coefficients showed some time dependence, reaching a plateau by 72 h. C15 was found to be an unexplained outlier. The 72 h results were:

C	12	14	15	16	18
Kd	3000± 80	8490± 920	3080± 270	23800 ±3200	78700 ±5400

Koc 17980 50830 - 143000 471000

log Koc 4.25 4.71 5.15 5.67
These data (neglecting the C15) can be interpreted as a QSAR in the usual way as:

Log Koc = 0.11 + 0.77 log Kow

R2 = 0.994

The result is in line with typical QSARs of this type.

Test substance: >= 95% 1-hexadecanol (36653-82-4); Linear alcohols labelled with 14-C, radiochemical purity 99%

Reliability: (2) valid with restrictions
Although not a SIDS end point, this study is considered to be the best study of Koc for these carbon numbers.

Reference: R. van Compernolle, D. McAvoy, A. Sherren, T. Wind, M.L. Cano, S.E. Belanger, P.B. Dorn, K.M. Kerr, "Predicting the sorption of fatty alcohols and alcohol ethoxylates to effluent and receiving water". Ecotox. and Environ. Safety, in press.

21-DEC-2005 (69)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)</u>

Media: water - soil
Method: other (calculation): various methods
Year: 2004

Method: Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 6.65 was used in the TGD calculation methods.

Result: TGD Hydrophobics method: Koc = 307000
TGD Non-hydrophobics method: Koc = 30100
TGD Alcohols method: Koc = 1240
SRC PCKOCWIN method: Koc = 3790

Test substance: 1-hexadecanol
Reliability: (2) valid with restrictions
The value was predicted using accepted calculation methods
Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.
28-DEC-2005 (5)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Type: Soil or sediment partition coefficient (Koc)
Test substance: 1-octadecanol
Method: Calculated using EPISUITE v. 3.10 and PCKOCWIN v. 1.66 using structural features of the molecule
Result: 12880
GLP: not applicable
Reliability: (2) valid with restrictions, calculated values
Reference: EPISUITE v. 3.10, U.S. Environmental Protection Agency, April 2001.

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Method: other (calculation):various methods
Year: 2004

Method: Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 7.75 was used in the TGD calculation methods.
Result: TGD hydrophobics method: Koc = 2390000
TGD Non-hydrophobics method: Koc = 112000
TGD Alcohols method: Koc = 3330
SRC PCKOCWIN method: Koc = 43800

Note: the TGD Alcohols method is valid up to log Kow = 5 and the Hydrophobics method is valid up to log Kow = 7.5. The results are presented for comparison only.
Test substance: 1-eicosanol (629-96-9)
Reliability: (2) valid with restrictions

The value was predicted using accepted calculation methods.

Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

28-DEC-2005 (3)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Method: other (calculation): various methods

Year: 2004

Method: Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The estimated log Kow value of 7.75 was used in the TGD calculation methods.

Result: TGD Hydrophobics method: Koc = 2390000
TGD Non-hydrophobics method: Koc = 112000
TGD Alcohols method: Koc = 3330
SRC PCKOCWIN method: Koc = 149000

Note: the TGD Alcohols method is valid up to log Kow = 5. and the Hydrophobics method is valid up to log Kow = 7.5. The results are presented for comparison only.

Test substance: 1-docosanol (661-19-8)

Reliability: (2) valid with restrictions
The value was predicted using accepted calculation methods.

Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

28-DEC-2005 (3)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Type: Soil or sediment partition coefficient (Koc)

Test substance: 1-tetracosanol (506-51-4)

Method: Calculated using EPISUITE v. 3.10 and PCKOCWIN v. 1.66 using structural features of the molecule

Result: 5.07×10^5

GLP: not applicable
Reliability: (2) valid with restrictions, calculated values
Reference: EPISUITE v. 3.10, U.S. Environmental Protection Agency, April 2001.

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Type: Soil or sediment partition coefficient (Koc)
Test substance: 1-hexacosanol (506-52-5)
Method: Calculated using EPISUITE v. 3.10 and PCKOCWIN v. 1.66 using structural features of the molecule
Result: 1.724×10^6
GLP: not applicable
Reliability: (2) valid with restrictions, calculated values
Reference: EPISUITE v. 3.10, U.S. Environmental Protection Agency, April 2001.

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Type: Soil or sediment partition coefficient (Koc)
Test substance: 1-octacosanol (557-61-9)
Method: Calculated using EPISUITE v. 3.10 and PCKOCWIN v. 1.66 using structural features of the molecule
Result: 5.866×10^6
GLP: not applicable
Reliability: (2) valid with restrictions, calculated values
Reference: EPISUITE v. 3.10, U.S. Environmental Protection Agency, April 2001.

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Type: Soil or sediment partition coefficient (Koc)
Test substance: 1-triacontanol (593-50-0)
Method: Calculated using EPISUITE v. 3.10 and PCKOCWIN v. 1.66 using structural features of the molecule
Result: 1.995×10^7
GLP: not applicable
Reliability: (2) valid with restrictions, calculated values
Reference: EPISUITE v. 3.10, U.S. Environmental Protection Agency, April 2001.

3.5 Biodegradation

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type Aerobic
Inoculum other: wastewater from domestic sewage
Contact time
Degradation = 74 (±) % after 5 day(s)
Result readily biodegradable

Kinetic of test subst.	5 day(s) = 74 % 10 day(s) = 74 % 15 day(s) = 95 % 20 day(s) = 84 %
Deg. product	
Method	other: BOD protocol 1974
Year	no data
GLP	no data
Test substance	ethanol (64-17-5)
Method	Biodegradability was measured in fresh water according to "standard methods for the examination of water and waste water" 13th Ed; American Public Health Association, New York, 1971.
Remark	Three concentrations tested (3, 7 and 10 mg/l) with at least two in duplicate. Tested concentrations gave a BOD of 3 to 30mg/l. Dissolved oxygen measured periodically (5 times in 20 days). Inoculum: wastewater from domestic sewage (assumed not adapted). COD measured.
Result	Measured COD was 1.99 mg O2/mg. Theoretical oxygen demand 2.1 mg/mg. (2) valid with restrictions
Reliability	Well reported study. Not to GLP and no test substance purity or source quoted.
Flag	Critical study for SIDS endpoint
Reference	Price, K.S. et al. (1974) Brine shrimp bioassay and seawater BOD of petrochemicals. J. Water Pollut. Control Fed. 46, 63 - 77.
19.10.2004	(67)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Aerobic
Inoculum	other: Filtered, settled domestic wastewater as seed in synthetic seawater
Contact time	
Degradation	75 (±) % after 20 day(s)
Result	readily biodegradable
Kinetic of test subst.	5 day(s) = 45 % 10 day(s) = 68 % 15 day(s) = 72 % 20 day(s) = 75 %
Deg. product	
Method	other: BOD protocol
Year	1974
GLP	no data

Test substance	ethanol (64-17-5)
Remark	Biodegradability measured in synthetic salt water according to "standard methods for the examination of water and waste water" 13th Ed. American Public Health Association, New York, 1971. Three concentrations tested (3, 7 and 10 mg/L). COD measured. Inoculum (other): Seed used was developed in seawater taken from Lavaca Bay, Texas. The seed was maintained by adding small amounts of settted raw wastewater periodically as a source of substrate. No further information available. Concentration of test chemical, vehicle, pre-acclimation conditions: 3, 7 and 10 mg/J ethanol was added using 0.1% stock solution. Temperature of incubation: Not specified. Dosing procedure: Not described. Domestic wastewater was placed in bottles to which was added aerated dilution water containing ethanol. Sampling frequency: BOD every 5 days; ethanol concentration was not monitored. Were appropriate controls and blank system used? Yes. Analytical method: Cumulative oxygen uptake in ethanol-amended and control samples was measured with dissolved O_2 meter. Method of calculating measured concentrations: Degradation rate was calculated as the % of theoretical oxygen demand utilized. Lag time: Not measured. Observed inhibition: Not measured. Excessive biodegradation: Not discussed. Excessive standard deviation: Not discussed. Time required for 10% degradation: Not discussed. At 5 days, 74% of ethanol had been degraded Total degradation at end of test: 84% .
Reliability	(2) valid with restrictions Well reported study. Not to GLP and no test substance purity or source quoted.
Reference	Price, K.S. et al. (1974) Brine shrimp bioassay and seawater BOD of petrochemicals. J. Water Pollut. Control Fed. 46, 63 - 77.
19.10.2004	(67)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Aerobic
Inoculum	activated sludge, domestic 500 mg/l related to
Contact time	
Degradation	= 37 (±) % after 1 day(s)
Result	readily biodegradable
Method	other
Year	1966

GLP	no data
Test substance	other TS: Analytical grade ethanol (64-17-5)
Remark	All sludges were capable of oxidizing ethanol as measured by BOD which was 37.3% of maximum and similar to that for other short-chain alcohols. Inoculum (other): Fresh activated sludge: activated sludges were obtained from municipal treatment plants in Columbus, Hilliard and Linworth, Ohio. Concentration of test chemical, vehicle, pre-acclimation conditions: 500 mg/L ethanol was added to 125 mL flasks containing 20 ml blended sludge with a concentration of 2500 mg/L suspended solids. Temperature of incubation: 20 deg C. Dosing procedure: see above. Sampling frequency: BOD 6, 12 and 24 h after inoculation. Ethanol concentrations were not measured. Were appropriate controls and blank system used? Yes. Analytical method: Oxygen uptake measured by Warburg respirometer. Method of calculating measured concentrations: Not discussed. Lag time: Not discussed. Observed inhibition: Not measured. Excessive biodegradation: Not discussed. Excessive standard deviation: Not discussed. Time required for 10% degradation: Not discussed. At 6 hours oxygen demand was 12.9% of theoretical. Total degradation at end of test: 37.3% at 24 hrs.
Reliability	(2) valid with restrictions
Reference	Gerhold, R. and Malaney, G. (1966). Structural determinants in the oxidation of aliphatic compounds by activated sludge. J. Water Poll. Control Fed. 38:562-579.
12.11.2004	(68)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Anaerobic
Inoculum	other: sediment and groundwater from methanogenic portion of shallow anoxic aquifer contaminated by landfill leachate
Concentration	50 mg/L related to Test substance
Contact time	30 day(s)
Degradation	= 91 (±) % after 30 day(s)
Result	readily biodegradable
Method	other
Year	1993
GLP	no data
Test substance	ethanol (64-17-5)
Method	Production of methane by ethanol-containing sediment was monitored by an

automated pressure transducer system.

Remark The acclimation period was 25-30 days.
Inoculum (other): Sediment and groundwater from a methanogenic portion of a shallow anoxic aquifer contaminated by landfill leachate.
Concentration of test chemical, vehicle, pre-acclimation conditions: 50 ppm C as ethanol. Ethanol was added to slurries of 50 g sediment and 75 mL groundwater in 160 mL bottles.
Temperature of incubation: Room temperature.
Dosing procedure: Not described.
Sampling frequency: Not described.
Were appropriate controls and blank system used? Yes, autoclaved controls.
Methane measurement: GC with flame ionization detector.
Method of calculating measured concentrations: Degradation rate was calculated as the mean of three tests.
Lag time: Acclimation period was 25-30 days.
Observed inhibition: Not discussed.

Excessive biodegradation: Not discussed.
Excessive standard deviation: Not discussed.
Time required for 10% degradation: Not discussed. (Rate calculated as 17.9 ppm C/day.
Total degradation at end oftest: 91% of theoretical CH4 production was recovered.
The rapidity and completeness of ethanol biodegradation is supported by the work of Corseuil et al, 1998 and by Yeh and Novak (1994) in both of which complete mineralization was achieved in aerobic or anaerobic conditions.
The rate of biodegradation was calculated to be 17.9 ppm C/day and total methane recovery was 91 % of the theoretical limit.

Result (2) valid with restrictions
No detailed results available, only final result reported.

Reliability Not GLP and no substance source or purity information.

Reference Suflita. J. and Monnile, M. (1993). Anaerobic biodegradation of known and potential gasoline oxygenates in the terrestrial subsurface. Environ. Sci. Technol. 27: 976-978.

19.10.2004 (69)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type Aerobic
Inoculum activated sludge
Contact time
Degradation = 96.8 (±2.4) % after 15 day(s)
Result readily biodegradable
Kinetic of test subst. 4 day(s) ca. 80 %

	8 day(s) ca. 88 % 11 day(s) ca. 100 % 15 day(s) ca. 92 % 20 day(s) ca. 98 %
Control Substance	Benzoic acid, sodium salt
Kinetic	1 day(s) ca. 10 % 5 day(s) ca. 70 %
Deg. product	
Method	OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO_2 evolution)"
Year	1991
GLP	no data
Test substance	ethanol (64-17-5)
Method	The mineral medium used was adopted from that recommended in the 1988 OECD Ring Test of Ready Biodegradability (OECD 301). Stock solutions based on demineralised water. Stock solution (d) used EDTA as a preservative. Since only about 1 % of cells in activated sludge are active it was considered that a 'cleaner' inoculum of similar activity could be obtained using secondary effluent from an activated sludge plant. The level of organic carbon introduced when using 10% by volume of secondary effluent to inoculate the test is only about 1-2 mg/litre. The test was therefore inoculated with secondary effluent from an activated sludge plant treating domestic sewage. The collected effluent was first passed through a coarse filter to remove gross particulate matter. The level of inorganic carbon in the inoculum was reduced before use by sparging with carbon dioxide-free air for about one hour while maintaining the pH at 6.5. The CO2 produced in the control vessels, using the maximum inoculum concentration of 10% secondary effluent, was in the range 0.4 - 1.3 mg/litre. Hence, in cases where positive results were obtained less than 10% of the carbon dioxide produced was derived from the control. The inoculum was not pre-adapted.
Remark	Using suitable volumetric apparatus 100±1 ml of the mineral salts media is dispensed into '125 ml' Hypo-Vial (Pierce Warriner (UK) Ltd.) The media is prepared so as to contain 0.5 to 10% by volume of inoculum and 2 to 10 mg/litre of test substance as organic carbon. Controls containing the same inoculum concentration but no test compound are also prepared. The vials are sealed with butyl rubber septa and aluminium crimp seals and placed on an orbital shaker in a temperature controlled environment. To follow the course of biodegradation and to statistically evaluate the extent of biodegradation on the final day of the

test a minimum of 12 vessels is required per test substance. This provides for a data point every fourth day and 4 replicates for the assessment of the final extent of biodegradation on the 28th day of the test.

A vessel is removed from the shaker as required, a sample of the headspace gas withdrawn using a gas syringe and the concentration of carbon dioxide determined. The seal is then broken and the concentration of dissolved inorganic carbon (DIC) in the solution is measured immediately. Similar determinations are made for a control vessel which does not contain the test substance. The difference in the total inorganic carbon found in the test and control vessels allows the quantity of carbon dioxide produced from the test compound to be ascertained.

Positive control: sodium benzoate.

The determination of carbon dioxide in both gaseous and aqueous samples was performed using a modified Ionics 555 TC- TOC Analyser. Carbon dioxide is released from aqueous samples of carbonate/bicarbonate by direct injection using a 0-200 dl Hamilton constant rate syringe onto an inert support loaded with phosphoric acid. The temperature in the reaction chamber is controlled at 150 degree C and pure nitrogen is used as the carrier gas. The detection system is a high sensitivity non-dispersive infra-red analyser. Gaseous samples are injected using a good quality gas-tight syringe.

The analyser is calibrated for the analysis of gaseous samples by injecting suitable volumes of a 0.25% v/v mixture of carbon dioxide in nitrogen. For liquid samples the instrument is calibrated using standard solutions of sodium hydrogen carbonate in the range 0 - 20 mgl/ as DCC.

Ethanol used as a comparator volatile compound in a study of the applicability of a modified form of the CO_2 production test for assessing ultimate biodegradability under aerobic conditions.

The test substance in a dilute mineral salts solution is incubated in seated vessels with appropriate micro-organisms for a period of up to 28 days.
Only about two thirds of the volume of the vessel is filled with liquid. At the test concentrations used only about 15% of the available oxygen in the headspace gas is required for the complete oxidation of all test compound carbon to carbon dioxide.

Any carbon dioxide produced by the breakdown of the test material is

	distributed between the liquid and gaseous phases. Periodically a vessel is taken, a sample of the headspace gas withdrawn using a gas syringe and the concentration of carbon dioxide In the headspace gas determined. The seal is then broken and the concentration of dissolved inorganic carbon (DOC) in the solution is measured. Similar determinations are made for a control vessel which does not contain the test substance. The difference in the total inorganic carbon found in the test and control vessels allows the quantity of carbon dioxide produced from the test compound to be ascertained. From a knowledge of the quantity of test material added and its carbon content the extent of mineralisation can be calculated.
Result	BOD28 Mean = 96.8%. SD 2.4 The method is shown to be compatible with existing techniques and is applicable to the testing of insoluble and volatile compounds. Reagent grade
Reliability	(2) valid with restrictions No temperature quoted for study and data only available in graphical form, otherwise well reported.
Reference	Birch, R.R., Fletcher, R.J. (1991) The application of dissolved inorganic carbon measurements to the study of aerobic biodegradability. Chemosphere 23 (7): 855-872.
19.11.2004	(70)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Aerobic
Inoculum	predominantly domestic sewage
Concentration	2 g/l related to test substance
Contact time	5 day(s) (±)
Degradation	
Test substance	ethanol (64-17-5)
Remark	Ethanol was used as a comparator substance in the description of a new potential test. Oxygen utilization was immediate and attained a high rate early in the test period. After 5 days the O2 uptake had passed the optimum rate and the slope of the O2 utilization curve matched that of the seed bank. Substrate utilization was demonstrated by a decrease in COD and TOC coincident with the rapid O2 uptake. Bacterial growth reached a peak level of over 10^6 organisms/ml on the third day of testing. Growth decreased thereafter to less than 10^4 organisms/ml at the end of the test.
Reliability	(4) not assignable
Reference	Young, R.H.F., Ryckman, D.W., Buzzell Jr, J. C. An improved tool for measuring biodegradability. J WPCF, 48(8) Pt. 2:R354-R368. (No year available; possibly 1978). (71)

19.10.2004

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type Anaerobic
Inoculum
Test substance ethanol (64-17-5)
Remark The anaerobic pseudo first order rate constants are published as follows:

ion	NO3(-)	Fe(3+)	SO4(2-)
rate constant	0.53	0.17	0.1

These are laboratory-derived values.
Reliability (4) not assignable
Reference Corseuil, et al., 1997; Aronson et al., 1997; USGS, 1998 andBarker et al., 1998 (full citations not available).
19.10.2004 (72)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Test substance ethanol (64-17-5)
Remark It is shown that 80-100 mg/l degrades aerobically in 5 days and anaerobically in 10-25 days.
Reliability (4) not assignable
Reference Kavanaugh, M.C; ,Stocking, A. (1999). Fate and Transport of Ethanol in the Environment.

US EPA Blue Ribbon Panel.
19.10.2004 (73)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Test substance ethanol (64-17-5)
Remark Ethanol is biodegraded in aerobic systems using activated sludge, sewage (including filtered and settled), wastewater,and soil inocula. Five day theoretical BOD values range from 37-86%. Anaerobic degradation (thermophilic digestion, 54 degree C) of ethanol (5 ml of a 5% aqueous ethanol solution) produced approximately 1000 ml gas/g sample using seed whichhad been prepared in a synthetic medium.

Reliability (4) not assignable
Reference Howard, P. (1990). Handbook of Environmental Fate and Exposure Data for Organic Chemicals, volume II. Solvents, Lewis Publishers: Chelsea, MI.
19.10.2004 (35)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Test substance	ethanol (64-17-5)
Remark	The aerobic half-life of ethanol in aqueous systems has been estimated to be between 6.5 and 26 hours, based upon a river die-away test for one sample of water from one river. The anaerobic half-life has been estimated to be between 26 and 104 hours based upon estimated unacclimated aqueous aerobic biodegradation half-life.
Reliability	(4) not assignable
Reference	Howard, P. (1990). Handbook of Environmental Fate and Exposure Data for Organic Chemicals, volume II. Solvents, Lewis Publishers: Chelsea, MI.
19.10.2004	(35)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Aerobic
Inoculum	activated sludge
Contact time	
Degradation	89 (±) % after 14 day(s)
Result	
Control Substance	Aniline
Kinetic of test subst.	
Test substance	ethanol (64-17-5)
Remark	Concentration of test substance: 100mg/l Concentration of activated sludge (as the concentration of suspended solid): 30mg/l Volume of test solution: 300ml Temperature: 25 degree C Initiation time before degradation started: 3 days
Reliability	(4) not assignable Results not available in detail and intermediate times only available in graphical form. No details of test method given although believed to be to an OECD protocol.
Reference	CERI, Japan (2003). http://qsar.cerij.or.jp/cgi-bin/DEGACC/index.cgi?E
19.10.2004	(74)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Method	other: modelled data
Test substance	ethanol (64-17-5)
Remark	BIOWIN v4.01 Results - predictions: Linear Model: Biodegrades Fast Non-Linear Model: Biodegrades Fast Ultimate Biodegradation Timeframe: Days-Weeks Primary Biodegradation Timeframe: Days

	Mill Linear Model: Readily Degradable
	Mill Non-Linear Model: Readily Degradable
Reliability	(4) not assignable
Reference	U.S. EPA URL http://www.epa.gov/opptintr/exposure/docs/episuite.htm
19.10.2004	(64)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Preferred study	
Type:	Aerobic biodegradation
Test Substance:	1-butanol (CAS No. 71-36-3)
Method:	APHA Standard Methods BOD (Standard Methods for the Examination of Water and Wastewater. 1971. 13th Ed. American Public Health Association, New York, NY) 20 day BOD (Biochemical Oxygen Demand) test Settled domestic wastewater (3 mL per bottle), unacclimated Three test chemical concentrations (3, 7, and 10 mg/L)
Results:	BOD5 6% ThOD (percent of theoretical oxygen demand) BOD10 87% ThOD BOD15 92% ThOD BOD20 92% ThOD
GLP:	No
Remark:	Readily biodegradable
Remark:	ThOD 2.59 g/g
Remark:	(2) valid with restrictions, not all typical study information was provided.
Reference:	Price KS, Waggy GT, Conway RA. 1974. Brine shrimp bioassay and seawater BOD of petrochemicals. J. Water Pollution Control Federation 46: 63-77.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Type:	aerobic saltwater
Inoculum:	w/raw sewage added (non-adapted)
Concentration:	3, 7, and 10 mg/L
Contact Time:	20 days
Degradation:	82% after 20 days
Results:	5 day = 45%, 10 day = 68%, 15 day = 71 %, 20 days 82%
Method:	BOD (Standard Methods for the Examination of Water and Wastewater. 1971. 13th Ed. American Public Health Association, New York, NY)
Year:	1971
GLP:	no data available
Test substance:	n-butanol
Remark:	Synthetic seawater screening study.
Reliability:	(2) valid with restrictions, not all typical study information was provided.
Reference:	American Public Health Association. 1971. Standard Methods for the Examination of Water and Wastewater. 1971. 13th Ed., New York, NY).

Price, K.S., G.T. Waggy, and R.A. Conway. 1974. Brine Shrimp Bioassay and Seawater BOD of Petrochemicals. J. Water Pollut. Contr. Fed. 46: 63-77.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test type: aerobic

Test medium: unadapted municipal sludge
Test method: Not Stated.
GLP: No

Test results: 36% of ThOD removed in 24 hrs.
Reliability: (2) valid with restrictions, not all study information available
Reference: Gerhold, R.M., Malaney, G.W. (1966) Structural determinants in the oxidation of aliphatic compounds by activated sludge. J. Water Pollut. Control Fed., 38 (4): 562-579.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test type: aerobic

Test medium: adapted municipal sludge
Test method: Not stated.
GLP: No

Test results: 44% of ThOD removed in 23 hrs.
Reliability: (2) valid with restrictions, not all study information available
Reference: McKinney, R.E., Jeris, J.S. (1955) Metabolism of low molecular weight alcohols by activated sludge. Sewage Ind. Wastes, 27(6): 728-735.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test type: aerobic

Test medium: fresh water
Test method: AFNOR Test
GLP: No

Test results: BOD_5 33% of ThOD.
Reliability: (2) valid with restrictions, not all study information available
Reference: Dore, M., Brunet, N., Legube, B. (1974) Participation de differerents

composes organiques a la valeur des crite.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 99.9% 1-butanol (71-36-3)
Test results: BOD_{10} 87% of ThOD.
Reliability: (2) valid with restrictions, not all study information available
Reference: Union Carbide Corporation. 1992b. Ecological Effects Data on Carbide Products and Process Chemicals. South Charleston, WV. 25303. (6.12.92).

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test type: aerobic

Test medium: fresh water-unadapted seed
Test method: Modified APHA Test
GLP: No

Test results: BOD_{20} 92% of ThOD.
Reliability: (2) valid with restrictions, not all study information available
Reference: Union Carbide Corporation. 1992b. Ecological Effects Data on Carbide Products and Process Chemicals. South Charleston, WV. 25303. (6.12.92).

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test type: aerobic

Test medium: adapted municipal sludge
Test method: ISO 8192
GLP: No

Test results: EC10 990 mg/l 30 min. test duration
Reliability: (2) valid with restrictions, not all study information available
Reference: BASF Corp, Internal Toxicology Report dated 9/10/91.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: aerobic
Inoculum: other: effluent of predominantly domestic sewage treatment plant
Concentration: 2 mg/l related to test substance 5 mg/l related to test substance
Contact time: 30 day(s)
Degradation: = 77 - 61 % after 30 day(s)
Result: readily biodegradable
Kinetic: 5 day(s) = 52 %

15 day(s) = 75 - 62 %
30 day(s) = 77 - 61 %

Control Subst.: other: Dodecylsulfate

Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1988
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Remark: The first value cited in the degradation and kinetic sections is for the 2 mg/l concentration while the second value is for the 5 mg/l concentration. Due to the low solubility of the test substance, a homogenous distribution was achieved by ultrasound dispersion and stabilization by an inert emulsifier. Although the present study does not include proof of the inertness, other studies from the same laboratory confirm this statement. The following validity criteria were met: (1) the parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level within 14 days, (3) oxygen depletion in the inoculum blank did not exceed 1.5 mg/l after 30 days, and (4) the residual concentration of oxygen in the test bottle did not fall below 0.5 mg/l at the lower test concentration. At the higher test concentration, the reported dissolved oxygen concentration was below 0.5 mg/l from Day 15 onwards.

Result: Kinetic of control substance: 5 days = 72%
15 days = 91%
30 days = 87%
The substance degraded >60% during the 10 day window and can be regarded as readily biodegradable.

Test condition: Concentration of inoculum: 1 ml/l (about 10E3 - 10E5 cells/ml)
Test volume: 290-296 ml
Temperature: 20 C
pH: not reported

Reliability: (2) valid with restrictions
The test was not conducted to GLP and did not meet one of the validity criteria for the test at the higher test concentration.

Flag: Critical study for SIDS endpoint

Reference: Richterich, K. 2002a. 1-Hexanol: Ultimate biodegradability in the closed bottle test. Final report R 0200259.

29-DEC-2005 (52)

<u>1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)</u>

Type: aerobic
Inoculum: other: no details provided on inoculum
Concentration: 20 mg/l related to Test substance
Contact time: 31 day(s)
Degradation: = 58 % after 31 day(s)
Result: inherently biodegradable
Kinetic: 4 day(s) = 35 %
10 day(s) = 49 %
17 day(s) = 55 %
24 day(s) = 57 %
31 day(s) = 58 %
Control Subst.: other: Sodium benzoate

Method: other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
Year: 1994
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Method: The inoculum used was activated sludge from a semi-continuous colony maintained in the laboratory. Incubation was carried out at 25°C in 200 ml Erlenmeyer flasks containing 5 µl of a alcohol and 100 ml of culture medium. Biodegradation rate constant was determined by measurement of the alcohol concentration in the supernatant of the culture by gas chromatography.
Remark: There is no information given on the validity criteria.
Result: Kinetic of control substance: 4 days = 47.1%
10 days = 58.1%
17 days = 60.5%
24 days = 61.2%
31 days = 62.2%
The test substance attained <60% degradation during the 10 day window. Sodium Benzoate was used as a positive control and reached a mineralization extent of 62.2%.
Test substance: The substance corresponds to CAS# 111-27-3.
Reliability: (4) not assignable
Non-guideline study.
Reference: Vista Chemical Company. 1994. Biodegradability of eleven VISTA ALFOL alcohols. TSR No. 6940-10-05-94.
17-OCT-2005 (78)

<u>1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)</u>

Type: aerobic
Inoculum: activated sludge

Method: other
Year: 1979
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Method: Incubation was carried out in 200 ml Erlenmeyer flasks containing 5 microlitres of alcohol and 100 ml of medium. Biodegradation rate constant was calculated from the time-course of the alcohol concentration in the supernatant of the culture. The concentration was analysed by gas chromatography.
Result: The biodegradation rate constant for Hexanol was 0.0799 hr-1. This equates to a half-life of 8.7 hours.
Reliability: (2) valid with restrictions
Not key study: Other studies with higher reliability score and more detailed data are available.
Reference: Yonezawa, Y. and Urushigawa, Y. 1979. Chemico-biological interactions in biological purification systems. V. Relation between biodegradation rate constants of aliphatic alcohols by activated sludge and their partition coefficients in a 1-octanol-water system. Chemosphere 3:139-142.
09-SEP-2005 (84)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: aerobic
Inoculum: other bacteria: municipal sewage treatment plant effluent
Concentration: 2 mg/l related to test substance
Degradation: = 77 % after 30 day(s)
Result: readily biodegradable

Test substance: >95% 1-hexanol (111-27-3)

Remark: Lorol C6
Source: Henkel KGaA.
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Assessment of data quality to current OECD standards is not possible and the study has therefore been assigned Reliability 4.
Reference: Henkel KGaA, unpublished data, Archive-No. 7198.

10-JAN-2005 (24)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: aerobic
Inoculum: activated sludge, domestic
Concentration: 20 mg/l related to Test substance
Contact time: 28 day(s)
Degradation: = 92 % after 28 day(s)
Result: readily biodegradable
Kinetic: 7 day(s) = 70 %
14 day(s) = 87 %
21 day(s) = 77 %
28 day(s) = 92 %
Control Subst.: Aniline

Method: other: ISO ring test "CO2 headspace biodegradation test"
Year: 1995
GLP: yes
Test substance: > 90% 1-octanol (111-87-5)

Remark: The following validity criteria were fulfilled
(1) the reference substance degraded by >60% after 14 days and
(2) the total inorganic carbon (TIC) present in the blank
controls at the end of the test was less than 15% of the
organic carbon added initially as the test substance. TIC at
Day 0 was not reported.
Result: Kinetic of control substance:
7 days = 62.0%
14 days = 94.2%
21 days = 87.3%
28 days = 114.7%
The test substance degraded >60% in the 10 day window. The
reference substance, aniline degraded by 89% after 28 days.
Test condition: Total solids concentration of the inoculum: not determined
Test volume: 80 ml
Temperature: 22 +/- 1 degree C
pH: 6.94 - 7.49.
Reliability: (2) valid with restrictions
Test is comparable to guideline study, although some
experimental details are not reported.
Flag: Critical study for SIDS endpoint
Reference: Procter & Gamble. 1996. Final report: ISO ring test CO2
headspace biodegradation test. Study ECM ETS 554/02.
11-OCT-2005 (92)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: aerobic
Inoculum: other: no information on inoculum provided
Concentration: 20 mg/l related to Test substance
Contact time: 31 day(s)
Degradation: = 60 % after 30 day(s)
Result: inherently biodegradable
Kinetic: 4 day(s) = 39 %
10 day(s) = 53 %
17 day(s) = 57 %
24 day(s) = 59 %
31 day(s) = 60 %
Control Subst.: other: Sodium benzoate

Method: other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
Year: 1994
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Method: This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 301B Modified Sturm Test) except that dichloromethane (30ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the solvent was evaporated leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
Remark: There is no information given on the validity criteria.
Result: Kinetic of control substance:
4 days = 47.1%
10 days = 58.1%
17 days = 60.5%
24 days = 61.2%
31 days = 62.2%
The test substance attained <60% degradation during the test period.
Reliability: (4) not assignable
The information reported is insufficient to assess the validity of this study.
Reference: Vista Chemical Company. 1994. Biodegradability of eleven VISTA ALFOL alcohols. TSR No. 6940-10-05-94.
11-OCT-2005 (123)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: aerobic

Inoculum: activated sludge, domestic, non-adapted
Concentration: 10 mg/l related to COD (Chemical Oxygen Demand)
Degradation: = 59 % after 29 day(s)
Result: inherently biodegradable
Kinetic: 3 day(s) = 15 %
8 day(s) = 43 %
15 day(s) = 52 %
29 day(s) = 59 %
Control Subst.: other: Sodium benzoate

Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year: 1996
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Method: A five-day bacterial inhibition test was performed under the conditions of the Closed Bottle Test. In this preliminary test, the test material was degraded to 27% of its COD. In a subsequent Modified Sturm Test, the test material was added to two vessels containing mineral salts medium and activated sludge to give a nominal test concentration of 10 mg C/L. Controls vessels comprised two containing inoculated mineral salts medium alone and one containing inoculated mineral salts medium plus sodium benzoate (positive control). Test and control vessels were aerated for 29 days with air treated to remove CO_2.
Remark: Cumulative CO_2 production in the controls after 29 days (77.8 and 80.1 mg CO_2) was within the acceptable range for this assay system (recommended maximum = 120 mg CO_2 for a three litre culture). The reference compound reached the pass level within 14 days and the parallel assays did not differ by more than 20%. No information is given on total inorganic carbon levels at the start of the test.
Mean cumulative CO_2 production by the mixtures containing the test substance at 10 mg C/L was equivalent to 15% after three days and 59% after 29 days.
Result: Kinetic of control substance:
3 days = 39%
8 days = 74%
15 days = 82%
29 days = 89%
The test substance degraded <60% over the test period and therefore cannot be considered readily biodegradable. However, significant degradation was observed therefore the substance is considered inherently biodegradable.

Test condition: Total solids concentration of inoculum: 30 mg/l
Temperature: 21.2 - 23.9°C
pH: 7.4 - 7.6
Reliability: (2) valid with restrictions
Guideline study although some validation data not reported.
Reference: Huntingdon Life Sciences Ltd. 1996a. Kalcohl 0898: Assessment of readily biodegradability. Modified Sturm Test. Report No. 96/KAS217/0325.
17-OCT-2005 (58)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: aerobic
Inoculum: other: effluent of predominantly domestic sewage treatment plant
Concentration: 50 mg/l related to COD (Chemical Oxygen Demand)
Contact time: 30 day(s)
Degradation: = 65 - 77 % after 30 day(s)
Result: readily biodegradable

Method: other: RDA-Blok-Test equivalent to a two-phase closed bottle test
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Remark: The method used is suitable for poorly water-soluble compounds. No information is provided regarding the validity criteria.
This information is from a summary of the full report and reports test concentration as 100 mg COD/L in the test procedure and 50 mg COD/L in the results section.
Result: 15 days = 30-75%
30 days = 65-77%
Degradation data only reported for days 15 and 30.
Reliability: (4) not assignable
Summary report only available. There is insufficient information reported to assess the validity of this test
Reference: Henkel KGaA. 1999i. 1-Octanol: Aerobic biodegradation: RDA-test according to Blok (AWU). Biological Research and Product Safety/Ecology: Unpublished results; test substance registration no. Fi 6369, test run no. 7.
30-AUG-2005 (53)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: aerobic

Inoculum: activated sludge

Method: other
Year: 1979
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Method: The inoculum used was activated sludge from a semi-continuous colony maintained in the laboratory.
Incubation was carried out at 25°C in 200 ml Erlenmeyer flasks containing 5 ul of a alcohol and 100 ml of culture medium.
Biodegradation rate constant was determined by measurement ofalcohol concentration in the supernatant of the culture by gas chromatography.
Result: The biodegradation rate constant for 1-octanol was 0.36 hr^{-1}.This equates to a half-life of 1.9 hours.
Reliability: (2) valid with restrictions
Non-guideline study.
Reference: Yonezawa, Y. and Urushigawa, Y. 1979. Chemico-biological interactions in biological purification systems. V. Relation between biodegradation rate constants of aliphatic alcohols by activated sludge and their partition coefficients in a 1-octanol-water system. Chemosphere 3:139-142.
30-AUG-2005 (128)

<u>1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)</u>

Type: anaerobic
Inoculum: other: digested sewage sludge diluted to 10%

Method: other
Year: 1983
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Method: Sludge was collected from primary or secondary anaerobic digesters. The method used digested sewage sludge diluted to 10% and incubated anaerobically in 160 ml serum bottles with 50 ug of C per ml of test chemical. Biodegradation was determined by the net increase in gas pressure in bottles with test chemicals over the pressure in nonamended sludge bottles. Gas production was measured by gas chromatography and by a pressure transducer. Compounds were incubated for 8 weeks.

Result: Octanol was readily mineralized (> 75% of theoretical methane production).
Test condition: Concentration of inoculum: 10% diluted sludge
Test volume: not reported
Temperature: 35 C
pH: not reported
Reliability: (2) valid with restrictions
Non-guideline study
Flag: Critical study for SIDS endpoint
Reference: Shelton, D.R. and Tiedje, J.M. 1984. General method for determining anaerobic biodegradation potential. Applied and Environmental Microbiology 850-857.
17-OCT-2005 (102)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: aerobic
Inoculum: activated sludge, adapted
Concentration: 2 mg/l related to Test substance
Degradation: = 100 % after 30 day(s)

Method: Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
GLP: no
Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Test condition: Biologically hard emulsifier used (Nonylphenol 10 EO/5 PO).
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Henkel KGaA, unpublished data (Registry No. 6369).
10-JAN-2005 (48)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: aerobic
Inoculum: other: municipal sewage treatment plant effluent
Concentration: 5 mg/l
Degradation: = 55 %

Method: Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"

GLP: no
Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Test condition: Biologically hard emulsifier used (Nonylphenol 10 EO/5 PO).
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Henkel KGaA, unpublished data (Registry No. 6369)
10-JAN-2005 (48)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: anaerobic
Inoculum: anaerobic sludge
Concentration: 50 mg/l related to Test substance

Method: ECETOC Anaerobic biodegradation
GLP: yes
Test substance: > 90% 1-octanol (111-87-5)

Remark: Mean degradation rate for 70 day test period was 64.6 +/- 19.2 %.
Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Henkel KGaA, unpublished data (Report No. RE 920219).
10-JAN-2005 (49)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: aerobic
Inoculum: other: effluent of predominantly domestic sewage treatment plant
Concentration: 2 mg/l related to Test substance
5 mg/l related to Test substance
Contact time: 30 day(s)
Degradation: = 88 % after 30 day(s)
Result: readily biodegradable

Kinetic: 5 day(s) =
15 day(s) = 74 %
30 day(s) = 88 %
Control Subst.: other: Dodecylsulfate

Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1983
GLP: no
Test substance: > 90% 1-decanol (112-30-1)
Remark: Due to the low water solubility of the test substance, a homogenous distribution was achieved by ultrasound dispersion and stabilization by an inert emulsifier. The dispersing agent was nonylphenol ethoxylate additionally propoxylated with 5 propyleneoxide units (NP 9,5 EO 5PO). The ratio of test substance to emulsifier was 1:1. The final concentrations of test substance were 2 and 5 mg/l.
The following validity criteria were met:
(1) the parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level within 14 days, (3) oxygen depletion in the inoculum blank did not exceed 1.5 mg/l after 30 days, and
(4) the residual concentration of oxygen in the test bottle did not fall below 0.5 mg/l at the lower test concentration. At the higher test concentration, the reported dissolved oxygen concentration was below 0.5 mg/l from Day 5 onwards.
Result: Kinetic of control substance:
5 days = 73%
15 days = 80%
30 days = 96%
The test substance (2 mg/l) attained >60% degradation within the 10 day window and can therefore be considered readily biodegradable. The values reported in the results section are for the 2 mg/l concentration. The 5 mg/l test concentration had insufficient residual dissolved oxygen content. The following results were given, 5 day >53%; 15 day >60%; 30 day >60%.
Test condition: Concentration of inoculum: 1 ml/l (about 10E3 - 10E5 cells/ml)
Test volume: 292.8 - 294.5 ml
Temperature: 20 degree C
pH: not reported
Reliability: (2) valid with restrictions
The test was not conducted to GLP and did not meet one of the validity criteria for the test at the higher test

concentration.
Flag: Critical study for SIDS endpoint
Reference: Richterich, K. 2002c. Lorol C 10-1-Decanol: Ultimate biodegradability in the closed bottle test. Final report R 0200257.
17-OCT-2005 (72)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: aerobic
Inoculum: other: effluent of predominantly domestic sewage treatment plant
Concentration: 50 mg/l related to COD (Chemical Oxygen Demand)
Contact time: 28 day(s)
Degradation: = 77 % after 30 day(s)
Result: readily biodegradable

Method: other
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Method: Biological Oxygen Demand Test for Insoluble Substances (BODIS). This method is based on the Closed Bottle Test (OECD test method 301D) and the RDA-Blok Test.
The test medium is inoculated with a mixed bacterial inoculum. After addition of a predetermined amount of test chemical (50 mg COD/l) the test vessels containing a known volume of aqueous test mixture (2/3) and air (1/3) are shaken continuously to assure steady state oxygen partitioning between liquid and gas phase. The degradation is followed by weekly measurements of the BOD in the aqueous phase during a 28-day period.
Remark: This information is from a summary of the full report. The test method used is based on OECD test method 301D and the RDA-Blok-Test. It is especially suitable for poorly water-soluble compounds. No information is provided regarding the validity criteria.
Result: 15 days = 55%
30 days = 77%
Report states Decanol is readily biodegradable, however insufficient information is provided to interpret the 10-d window acceptability criterion.
Reliability: (4) not assignable
Summary report only available. There is insufficient information reported to assess the validity of this test.
Reference: Henkel KGaA. 1999c. 1-Decanol: Aerobic biodegradation: BODIS test/ Two-phase closed bottle test. Biological

Research and Product Safety/Ecology: Unpublished results;
test substance registration No. 6368, test run No. 8.
05-OCT-2005 (43)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: aerobic
Inoculum: other: no details provided on inoculum
Concentration: 20 mg/l related to Test substance
Contact time: 31 day(s)
Degradation: = 54 % after 31 day(s)
Result: inherently biodegradable
Kinetic: 4 day(s) = 32 %
10 day(s) = 46 %
17 day(s) = 51 %
24 day(s) = 53 %
31 day(s) = 54 %
Control Subst.: other: Sodium benzoate

Method: other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
Year: 1994
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)
Method: This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 301B Modified Sturm Test) with one exception: after the samples were added, dichloromethane (30ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the solvent was evaporated leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
Remark: No information is provided regarding the validity criteria.
Result:
The test substance attained <60% degradation during the test period and therefore cannot be considered readily biodegradable.
Kinetic of control substance: 4 days = 47.1%
10 days = 58.1%
17 days = 60.5%
24 days = 61.2%
31 days = 62.2%
Reliability: (4) not assignable
The information reported is insufficient to assess the validity of this study.
Reference: Vista Chemical Company. 1994. Biodegradability of eleven

VISTA ALFOL alcohols. TSR No. 6940-10-05-94.
05-OCT-2005 (101)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: aerobic
Inoculum: activated sludge, domestic, non-adapted
Concentration: 10 mg/l related to COD (Chemical Oxygen Demand)
Contact time: 29 day(s)
Degradation: = 29 % after 29 day(s)
Result: other: not readily biodegradable
Kinetic: 5 day(s) = 18 %
15 day(s) = 26 %
29 day(s) = 29 %
Control Subst.: other: Sodium benzoate

Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year: 1996
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Method: A five-day bacterial inhibition test was performed under the conditions of the Closed Bottle Test. In a subsequent Modified Sturm Test, the test material was added to two vessels containing mineral salts medium and activated sludge to give a nominal test concentration of 10 mg C/L. Control vessels comprised two containing inoculated mineral salts medium alone and one containing inoculated mineral salts plus sodium benzoate (10 mg C/L). Test and control vessels were aerated for 29 days with air that had been treated to remove CO_2.
Remark: Cumulative CO_2 production in the controls after 29 days (77.8 and 80.1 mg CO_2) was within the acceptable range for this assay system (recommended maximum = 120 mg CO_2 for a three litre culture). The reference compound reached the pass level within 14 days and the parallel assays did not differ by more than 20%. No information is given on total inorganic carbon levels at the start of the test.
Result: The test substance attained <60% degradation during the test period therefore it cannot be considered readily biodegradable.
Kinetic of control substance: 5 days = 61%
15 days = 82%
29 days = 89%
Test condition: Total solids concentration of inoculum: 30 mg/l

Temperature: 21.2 - 23.9°C
pH: 7.4 - 7.6
Reliability: (2) valid with restrictions
Guideline study although some validation data not reported.
Reference: Huntingdon Life Sciences Ltd. 1996b. Kalcohl 1095: Assessment of readily biodegradability. Modified Sturm Test. Report No. 96/KAS223/0327.
09-SEP-2005 (47)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: aerobic
Inoculum: other: municipal sewage treatment plant effluent
Concentration: 2 mg/l related to Test substance
Degradation: = 86 % after 30 day(s)
Result: readily biodegradable

Method: Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
Test substance: > 90% 1-decanol (112-30-1)

Remark: Values corrected for control (emulsifier alone). parameter: % BOD/COD
Source: Henkel KGaA Duesseldorf
Test condition: Biologically hard Nonylphenol 10EO/5PO used as emulsifier.
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Henkel KGaA, unpublished data (Registry No. 6368).
10-JAN-2005 (34)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: aerobic
Inoculum: domestic sewage, adapted
Degradation: = 36.3 % after 5 day(s)

Method: other: 5 day BOD according to "Standard Methods for the
Year: 1980
Test substance: > 90% 1-decanol (112-30-1)
Source: Henkel KGaA Duesseldorf
Test condition: 21 +/- 3 degr. C, parameter: BOD5 [mmole/mmole substrate]/ BOD theoretical. Microbial culture from domestic sewage

adapted to test substance prior to test.
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Babeu, L. & Vaishnav, D.D., J. Ind. Microbiol. 2, 107-115 (1987); Vaishnav, D.D. et al. Chemosphere 16 (1987), 695-703.
10-JAN-2005 (8)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: aerobic
Inoculum: other: sewage treatment plant effluent/biological stage
Concentration: 2 mg/l
Degradation: = 66 - 80 % after 30 day(s)
Result: readily biodegradable

Method: Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
Test substance: > 90% 1-decanol (112-30-1)

Remark: Original experimental data: erheblich getrübte Stammlsg. Lösungsvermittler eingesetzt ungenügender Restsauerstoff in der höheren Prüfkonzentration.
Source: Henkel KGaA Duesseldorf
Test condition: #1: 2 mg/l referring to Active Substance: 86% with parameter % BSB/CSB
#2: 5 mg/l referring to Active Substance: 60% with parameter % BSB/CSB
Test substance: Analogy; data taken from CASRN 112-30-1 <1-Decanol>, Active Matter = 100 %.
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Henkel KGaA, unpublished data, File 59, Page/Assay 691.

Henkel KGaA, unpublished data, Final report 1984 2277.

Henkel KGaA, unpublished data, Protocol 32, Page/Assay 691.
28-SEP-2005 (36) (37) (39)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type: aerobic
Inoculum: other: effluent of predominantly domestic sewage treatment plant
Concentration: 2 mg/l related to Test substance
Contact time: 28 day(s)
Degradation: = 79 % after 28 day(s)
Result: readily biodegradable

Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1992
GLP: yes
Test substance: Dodecanol (112-53-8)

Method: EEC-Directive 92/69/EEC Annex V, Part C: Methods for the Determination of ecotoxicity. C.4. Biodegradation: determination of the 'ready biodegradability' C.4-E
This method corresponds to OECD test method 301D.
Remark: The following validity criteria were fulfilled (1) the reference substance reached the pass level of 60% within 14 days. (2) Parallel assays did not differ by greater than 20%. (3) Residual concentration of O2 in test bottles did not fall below 0.5 mg/l. (4) O2 depletion in the blanks was less than 1.5 mg/l after 29 days.
Result: 7 days = 54%
14 days = 68%
21 days = 80%
28 days = 79%
The test substance (2 mg/l) attained >60% degradation during the 14 day window. The values reported in the results section are for the 2 mg/l concentration. The 5 mg/l concentration of test substance had insufficient residual dissolved oxygen content after 21 days.
Source: Richterich 1993.
Test condition: INOCULUM/TEST ORGANISM
Sampling site: Plant Hochdahl, Germany
INITIAL TEST SUBSTANCE CONCENTRATION: 2 and 5 mg/l
METHOD OF PREPARATION OF TEST SOLUTION: an inert emulsifier (nonylphenol ethoxylated propoxylated, NP+9.5 EO+5PO) was used to disperse the test substance. Concentration of emulsifier not reported.
ANALYTICAL PARAMETER: Chemical Oxygen Demand (COD)
TEST CONDITIONS:
- Composition of medium: not reported

- Additional substrate: none
- Test temperature: 20 +/- 1C
- pH value: not reported
- Aeration of dilution water: not reported
- Concentration of suspended solids: not reported

INTERMEDIATES/DEGRADATION PRODUCTS: not reported
NITRATE/NITRITE MEASUREMENT: yes
CONTROLS: mineral medium/ mineral medium with inoculum/ mineral medium with inoculum and emulsifier. Degradation rate of test substance was corrected by oxygen uptake of blank inoculum and emulsifier control.
REFERENCE SUBSTANCE: Sodium benzoate

Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
Reference: Richterich. 1993. 1-Dodecanol: Aerobic biodegradation: Closed bottle test. Biological Research and Product Safety/Ecology: Unpublished results; test substance registration no. SAT 910724, Henkel KGaA; Report No. RE 920247 (With English summary report no. R9901416).
03-NOV-2003 (17)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type: aerobic
Inoculum: activated sludge
Concentration: 100 mg/l related to COD (Chemical Oxygen Demand)
Degradation: = 100 % after 28 day(s)
Result: readily biodegradable

Method: other: ISO 10708 (BODIS)
Year: 1992
GLP: yes
Test substance: dodecanol (112-53-8)

Method: The test method used is based on OECD test method 301D and the RDA-Blok-Test. It is especially suitable for poorly water-soluble compounds. The test medium is inoculated and the test chemical added. The test vessels are then closed and shaken continuously. Weekly measurements of the BOD from the aqueous phase are taken.
Remark: Total oxygen uptake in flasks is calculated from blank-corrected decrease in measured dissolved oxygen concentration divided by saturation value at normal conditions and multiplied with total oxygen content originally present in liquid and gas phase.
The following validity criteria are met (1) Parallel assays

did not differ by more than 20%, (2) reference compound reached the pass level within 14 days and (3) residual concentration of oxygen did not fall below 0.5 mg/l. It could not be determined whether oxygen depletion in the blank exceeded 1.5 mg/l after 28 days as no data for day 0 was included.

Result: 7 days = 72%
14 days = 89%
21 days = 93%
28 days = 100%
The substance degraded >60% in the 10 day window. The reference substance, Sodium acetate trihydrate, degraded 86% over the 28 day period.

Source: Henkel KGaA 1992c.

Test condition: Concentration of activated sludge: 30 mg dry matter/l
Test volume: 200 ml
Temperature: 20-25 C
pH: not reported

Test substance: This test substance corresponds to CAS # 112-53-8. Tradename is Lorol C12-99.

Reliability: (1) valid without restriction
Not key study: Other study with same reliability score and using OECD 301D methodology exists.

Reference: Henkel KGaA. 1992c. Lorol C12-99: Bewertung der biologischen Abbaubarkeit im BODIS-test. TFB-okologi RE 920025.

29-OCT-2003 (8)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)</u>

Type: aerobic
Inoculum: activated sludge, domestic, non-adapted
Concentration: 20 mg/l related to test substance
Contact time: 46 day(s)
Degradation: = 71 % after 28 day(s)
Result: readily biodegradable

Method: other: Sturm 1973
Year: 1991
GLP: no data
Test substance: dodecanol (112-53-8)
Method: This test method corresponds to OECD 301B
Remark: The following validity criteria were met: (1) the blanks were valid for this test, the maximum milligrams of carbon dioxide were well within the 40 mg/l range, (2) both sodium acetate samples obeyed the 10-60% rule, no days were

required for the bacterial population to acclimate to the sodium acetate, (3) Parallel assays did not differ by more than 20%.

Result: 4 days = 16%
8 days = 44%
14 days = 60%
28 days = 71%
46 days = 73%
Report states that both ALFOL 12 alcohol samples obeyed the '10-day window' rule and 3 days were required for the bacterial population to acclimate to the alcohol. The reference substance, Sodium acetate, degraded by 78% after 28 days.

Source: Morris et al. 1991.

Test substance: The test substance corresponds to CAS# 112-53-8. Tradename is Alfol 12.

Reliability: (2) valid with restrictions
Not key study: Other studies with higher reliability score and a with higher degradation rate are available.

Reference: Morris, P.A., Filler, P.A., and Nielsen, A.M. 1991. Sturm test evaluation of Alfol 1618-CG alcohol, Alfol 12 alcohol, Alfonic 1618-87 alcohol ethoxylate, and ditallow dimethyl ammonium methyl sulfate quaternary amine. Vista Chemical Company research report No. 6911-34-5-91.

25-SEP-2003 (16)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)</u>

Type: aerobic
Inoculum: activated sludge, domestic
Concentration: 26 mg/l related to test substance
Degradation: = 50 % after 28 day(s)
Result: inherently biodegradable

Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year: 1996
GLP: yes
Test substance: Dodecanol (112-53-8)

Method: Test solutions were prepared and inoculated in 5 L glass vessels each containing 3 litres of solution. Each test vessel was inoculated with the prepared inoculum at a final concentration of 30 mg suspended solids (ss)/l. The study was carried out at a temperature of 21 degree C in darkness.

Remark: The following validity criteria were met (1) the IC content

of the test substance suspension in the mineral medium at the beginning of the test was less than 5% of the total carbon, (2) parallel assays did not differ by more than 20%, (3) reference compound reached the pass level within 14 days, (4) Total CO2 evolution in the inoculum blank did not exceed 40 mg/l at the end of the test.

Result: 6 days = 8%
14 days = 27%
20 days = 48%
28 days = 50%
The test substance degraded <60% during the 10 day window. The reference substance, Sodium benzoate degraded by 105% after 28 days.

Source: Mead 1997a.

Test substance: This substance corresponds to CAS# 112-53-8. Tradename is Kalcol 2098.

Reliability: (1) valid without restriction
Not key study: Other studies (same reliability score) but with higher degradation rate are available.

Reference: Mead, C. 1997a. Kalcohl 2098: Assessment of ready biodegradability; CO2 Evolution Test. SLP Project Number 140/591.

10-SEP-2003 (15)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type: aerobic
Inoculum: other: no information provided on inoculum
Concentration: 20 mg/l related to test substance
Contact time: 31 day(s)
Degradation: = 41 % after 31 day(s)
Result: inherently biodegradable

Method: other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
Year: 1994
GLP: no data
Test substance: dodecanol (112-53-8)

Method: This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 301B Modified Sturm Test) with one exception: after the samples were added, dichloromethane (30ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the solvent was evaporated

leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.

Remark: There is no information given on the validity criteria.

Result: 4 days = 11%
10 days = 26%
17 days = 34%
24 days = 38%
31 days = 41%
The test substance attained <60% degradation during the 10 day window. Sodium benzoate was used as a positive control and reached a mineralization extent of 62.2%.

Source: Vista 1994.

Test substance: The substance corresponds to CAS# 112-53-8. Tradename is ALFOL 12.

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) but with higher degradation rates are available.

Reference: Vista Chemical Company. 1994. Biodegradability of eleven VISTA ALFOL alcohols. TSR No. 6940-10-05-94.

18-SEP-2003 (27)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)</u>

Type: aerobic

Inoculum: other: activated sludge, predominantly domestic

Concentration: 100 mg/l related to COD (Chemical Oxygen Demand)

Contact time: 28 day(s)

Degradation: = 92 % after 28 day(s)

Result: readily biodegradable

Kinetic: 7 day(s) = 67 %
14 day(s) = 84 %
21 day(s) = 88 %
28 day(s) = 92 %

Control Subst.: other: Sodium acetate

Method: other: ISO 10708 (BODIS)

Year: 1992

GLP: yes

Test substance: > 95% 1-tetradecanol (112-72-1)

Method: The test method used is based on OECD test method 301D and the RDA-Blok-Test. Mineral medium was inoculated with activated sludge and stabilized for one week at 20-25 degree C with continuous stirring. After stabilisation, 200 ml of test medium was filled into 300 ml bottles, aerated until O2 saturation was reached and spiked with test substance by

directly weighing into the test vessels. Vessels were filled 2/3, stoppered and shaken continuously at 20-25 C.

Degradation was followed by weekly measurements of BOD using an O2-electrode. Oxygen consumption resulting from biodegradation of the test substance was corrected by oxygen uptake of blank inoculum. Degradation rate was calculated as % BOD/COD.

Remark: The validity criteria were fulfilled:
(1) degradation rate of reference has reached level of 60% within 14 days,
(2) Parallel assays did not differ by more than 20%,
(3) total oxygen consumption in blanks after first week was lower than 3 mg O2 and lower 1 mg O2 in the following weeks and
(4) residual concentration of O2 in the test bottles did not fall below 0.5 mg/l.

Result: Kinetic of control substance:
7 days = 75%
14 days = 85%
21 days = 86%
28 days = 86%
The test substance attained >60% degradation within the 10-day window, therefore it can be considered readily biodegradable.

Test condition: Concentration of activated sludge: 30 mg dry matter/l
Test volume: 200ml
Temperature: 20-25 C
pH: not reported

Reliability: (1) valid without restriction

Flag: Critical study for SIDS endpoint

Reference: Henkel KGaA. 1992d. Lorol C14-98. Bewertung der biologischen Abbaubarkeit im BODIS-test. Biological Research & Product Safety/Ecology Department. Report No. 920026 (test substance registration no. SAT 910723, test run no. 118). 5 Marz 1992.

17-OCT-2005 (37)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)</u>

Type: aerobic

Inoculum: other: no information provided on inoculum

Concentration: 20 mg/l related to test substance

Contact time: 31 day(s)

Degradation: = 57 % after 31 day(s)

Result: inherently biodegradable

Kinetic: 4 day(s) = 28 %
10 day(s) = 47 %

17 day(s) = 54 %
24 day(s) = 56 %
31 day(s) = 57 %
Control Subst.: other: Sodium benzoate

Method: other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
Year: 1994
GLP: no data
Test substance: > 95% 1-Tetradecanol (112-72-1)

Method: This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 310B Modified Sturm Test) with one exception: after the samples were added, dichloromethane (30ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the solvent was evaporated leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
Remark: There is no information given on the validity criteria.
Result: Kinetic of control substance:
4 days = 47.1%
10 days = 58.1%
17 days = 60.5%
24 days = 61.2%
31 days = 62.2%
The test substance attained <60% degradation over the test period, therefore it cannot be considered readily biodegradable.
Reliability: (4) not assignable
The information reported is insufficient to assess the validity of this study.
Reference: Vista Chemical Company. 1994. Biodegradability of eleven VISTA ALFOL alcohols. TSR No. 6940-10-05-94.
17-OCT-2005 (79)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)</u>

Type: aerobic
Inoculum: activated sludge, domestic, non-adapted
Concentration: 25.4 mg/l related to Test substance
Degradation: = 28 % after 28 day(s)
Result: other: not readily biodegradable
Kinetic: 1 day(s) = 2 %
10 day(s) = 10 %
20 day(s) = 23 %
28 day(s) = 28 %

Control Subst.: other: Sodium benzoate

Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year: 1996
GLP: yes
Test substance: > 95% 1-Tetradecanol (112-72-1)

Remark: The following validity criteria were met
(1) Parallel assays did not differ by more than 20%,
(2) the reference substance degraded by >60% during the 14 day window,
(3) CO2 evolution in the inoculum blank did not exceed 40 mg/l at the end of the test,
(4) IC content of the test substance suspension in mineral medium at the start of the test was less than 5% of the total carbon.
Result: Kinetic of control substance:
1 days = 20%
10 days = 66%
20 days = 91%
28 days = 105%
The test substance attained <60% degradation over the test period, therefore it cannot be considered readily biodegradable.
Test condition: Concentration of activated sludge: 30 mg dry matter/l
Test volume: 3 L
Temperature: 21°C
pH: not reported
Reliability: (1) valid without restriction
Not key study: Other studies (same reliability score) but with higher degradation rate are available.
Reference: Mead, C. 1997b. Kalcohl 4098: Assessment of readily biodegradability; CO2 evolution test. SPL Project Number 140/598.
17-OCT-2005 (48)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)</u>

Type: aerobic
Inoculum: activated sludge, domestic
Concentration: 50 mg/l
Degradation: = 55 - 66 % after 28 day(s)

Method: ISO Draft "BOD Test for insoluble substances"
Test substance: > 95% 1-tetradecanol (112-72-1)

Method: two-phase closed bottle test
Remark: Abbauhemmtest: keine Effekte. Animpfung 10 fach höher als Routine BLOK Test (hohe Eigenzehrung IZK) parallel wurde ein Hemmtes durchgeführt CSB= 2.18mg O2/mg AS BSBT=3.14mg O2/mg AS
Source: Henkel KGaA Duesseldorf
Test condition: #1: 50 mg/l referring to Chemical oxygen demand: 55% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 66% with parameter % BSB/ThSB
#3: 50 mg/l referring to Chemical oxygen demand: 63% with parameter % BSB/CSB
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Henkel KGaA, unpublished data, File 5, Page/Assay 29

Henkel KGaA, unpublished data, Protocol 1, Page/Assay 29
11-OCT-2005 (29) (35)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Type: aerobic
Inoculum: activated sludge, domestic
Concentration: 50 mg/l
Degradation: = 40 - 58 % after 28 day(s)

Method: ISO Draft "BOD Test for insoluble substances"
Test substance: > 95% 1-tetradecanol (112-72-1)
Method: two phase closed bottle test
Remark: Abbauhemmtest: keine Effekte.
Source: Henkel KGaA Duesseldorf
Test condition: #1: 50 mg/l referring to Chemical oxygen demand: 58% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 40% with parameter % BSB/ThSB
#3: 50 mg/l referring to Chemical oxygen demand: 68% with parameter % BSB/CSB
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Henkel KGaA, unpublished data, File 5, Page/Assay 30

Henkel KGaA, unpublished data, Protocol 1, Page/Assay 30
28-SEP-2005 (30) (36)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Type: aerobic
Inoculum: other: sewage treatment plant effluent/biological stage
Concentration: 50 mg/l
Degradation: = 80 - 82 % after 30 day(s)
Result: other: : well biodegradable

Method: other: RDA-Test according to Blok (AWU)
Test substance: > 95% 1-Tetradecanol (112-72-1)

Remark: Parallel wurde eine Testreihe ohne Zwischenbelüftung geprüft 74-80% BSB30/BSBT ungenügend Restsauerstoff CSB= 2.18 mg O2/mg AS BSBT=3.14mg O2/mg AS
Source: Henkel KGaA Duesseldorf
Test condition: #1: 50 mg/l referring to Chemical oxygen demand: 82% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 80% with parameter % BSB/ThSB
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Henkel KGaA, unpublished data, File 5, Page/Assay 27

Henkel KGaA, unpublished data, Final report 1986 2415

Henkel KGaA, unpublished data, Protocol 1, Page/Assay 27
11-OCT-2005 (27) (31) (33)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Type: aerobic
Inoculum: other: sewage treatment plant effluent/biological stage
Concentration: 50 mg/l
Degradation: = 91 - 91 % after 30 day(s)
Result: other: well biodegradable

Method: other: RDA-Test according to Blok (AWU)
Test substance: > 95% 1-tetradecanol (112-72-1)

Remark: Parallel wurde eine Testreihe ohne Zwischenbelüftung geprüft 83% BSB30/BSBT ungenügend Restsuerstoff CSB= 2.18mg O2/mg AS BSBT=3.14mg O2/mg AS

Source: Henkel KGaA Duesseldorf

Test condition: #1: 50 mg/l referring to Chemical oxygen demand: 91% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 91% with parameter % BSB/ThSB

Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

Reference: Henkel KGaA, unpublished data, File 5, Page/Assay 28

Henkel KGaA, unpublished data, Final report 1986 2415

Henkel KGaA, unpublished data, Protocol 1, Page/Assay 28

11-OCT-2005 (28) (31) (34)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Method: Laboratory continuous activated sludge study.

4 mg/L of TS
20ºC
Hydraulic residence time (HRT) 6 h
Sludge retention time (SRT) 10 d

The feed to the sludge unit was of sterile synthetic sewage and AE concentrate and non-sterile tap water.

19 d acclimation was used, followed by 10 days of evaluation. At the start the unit was seeded with sewage treatment plant (STP) activated sludge.

The unit was sampled several times per week, and the samples were analysed immediately.

Analytical recovery of the alcohols was high.

The results showed that the CAS unit was running in a similar way to a full scale STP.

Remark: This paper describes mainly the properties of alcohol

ethoxylates (AE) but contains valuable data about the properties and environmental exposures of alcohols themselves. This study should not be considered as a study of alcohols alone, but is important in that it indicates that the extent of removal of alcohols from an exposure route that can be anticipated. This extent is high. The waste water organisms were exposed principally to ethoxylates, but the alcohols would be generated by the degradation of the ethoxylates.

Result: Results are corrected for control values.

Alcohol	Conc. in effluent ng/L	Conc. in sludge µg/g	%removal
C12	18	0.6	98.6
C13	21	0.7	99.5
C14	5.5	0	99.6
C15	2.9	1.1	99.8
C16	1.6	0.01	99.5
C18	58	0.7	99.1
Total	130	2	99.4

Total elimination of ethoxylates 97.4
Total in waste sludge solids 2.0
Total in suspended solids 0
This shows that most of that which does not degrade (itself a small amount) is in the solids.

Test substance: 2:1 mixture of NEODOL 25-7 and GENAPOL T110

Alkyl chain distribution

C	Mol ratio
12	1
13	2
14	2.3
15	1.8
16	1.1
18	2.9

Reliability: (2) valid with restrictions
OECD 303. Public domain paper based on a fuller Shell laboratory report.

Reference: T. Wind, R.J. Stephenson, C.V. Eadsforth, A. Sherren, R. Toy. Ecotox and Environ Safety, in press. Determination of the fate of alcohol ethoxylate homologues in a laboratory continuous activated sludge unit.

21-DEC-2005 (72)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)</u>

Method: The study was a batch-mode activated sludge die-away system. Two treatments consisting of 1 litre each of biologically active sludge were prepared for each test substance. The 14-C alcohols were dissolved in methanol, which was diluted in water and dosed into the sludge in 2-litre flasks.

Disappearance of parent, formation and disappearance of metabolites, uptake into biomass and mineralization to 14-C CO2 were monitored over time.

Activated sludge from a municipal WWTP was obtained, and used at 2500 mg/L.

The TS was dosed at 0.05 µM: this is equivalent to 9.3µg/L (C12), 10.0 µg/L (C14), 10.7 µg/L (C16); added to flasks at 20ºC.

Remark: The results for three substances are considered alongside each other since the results of the whole study are useful to show the consistency of the results.

Result: Recoveries were high.

After 48h incubation:

C	Parent	metabolites	Water	Solids	CO2
C12	0.8	5.9	3.5	20.7	73.9
C14	1.3	6.3	2.0	21.0	76.7
C16	2.6	11.5	2.1	17.0	65.3

Concentrations were modelled with the equation
C = Ae^(-k1t) + B(e^-k2t)
(a two compartment first order decay model)

%	A	k1 h-1	B	k2 h-1
C12	82±2	113±8	9±1	0.36±0.1
C14	82±2	87±5	12±1	0.30±0.1
C16	41±3	103±23	48±2	0.43±0.04

The results show the high biodegradability of C12 to 16 alcohols in activated sludge.

Test substance: Radiolabelled (14C) C12, C14 and C16 alcohols.

Reliability: (2) valid with restrictions
Non-standard study conducted to a scientifically sound method.

Reference: T.W. Federle, N.R. Itrich, 'Fate of Free and linear alcohol-ethoxylate-derived fatty alcohols in activated

sludge'. Ecotox. Environ. Safety, in press.

21-DEC-2005 (73)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)

Method: Effluent monitoring of waste water treatment plants receiving predominantly municipal effluent. Concentration of alcohols and alcohol ethoxylates were measured.

Twenty-four hour composite samples of influent and effluent were collected from each of the locations from three days. They were preserved with formalin at the time of collection. These were composited in proportion to flow.

Samples of 4 litres were obtained and extracted onto a succession of cartridges, followed by solvent elution. Quantitative analysis of the eluates was by a derivitisation Liquid-chromatography-mass spectrometric (LCMS) technique.

Result: Influent (In), effluent (Eff) values in µg/l, and % removal of alcohols are indicated in the table below, with alcohol data considered in two groups. The State in which the WWTP is found is indicated by the usual 2-letter abbreviation.

	C12-15 OH			C16-18 OH		
WWTP type	In	eff	%	in	eff	%
TX Lagoon	297	2	99.3	92.7	2.4	97.4
NJ Oxidation Ditch	249	0.7	99.7	181	0.8	99.6
OH Rotating biological contactor	157	0.1	0.06	77	0.07	99.9
IA Trickling filter	499	2.0	99.6	354	2.3	99.4
MO Trickling filter	532	4.9	99.1	315	9	97.3
KS Lagoon	67.5	1.1	98.4	35.4	2.2	93.8
CA Activated sludge	20.05	0.2	99.9	169	0.4	99.8
OR Activated	92.9	0.2	99.8	133	0.6	99.5

sludge

AZ Oxidation 702 0.3 100 394 0.5 99.9
ditch

Results for the carbon number groups are considered alongside each other to enable the context of every data point to be seen. In the overall interpretation of the data, the results have been used with those from other studies to determine the contribution of measured alcohol concentrations from various sources.

Reliability: (2) valid with restrictions
Non-GLP studies conducted to a high standard.

Reference: S.W. Morrall, J.C. Dunphy, M.L. Cano, A. Evans, D.C. McAvoy, B.P. Price, W.S. Eckhoff. 'Removal and environmental exposure of alcohol ethoxylates in US sewage treatment', Ecotox.Environ Safety, in press.

21-DEC-2005 (58)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: aerobic
Inoculum: activated sludge, domestic
Concentration: 17.1 mg/l related to Test substance
Contact time: 29 day(s)
Degradation: = 62 % after 28 day(s)
Result: other: not readily biodegradable
Kinetic: 6 day(s) = 10 %
16 day(s) = 52 %
28 day(s) = 62 %
Control Subst.: other: Sodium benzoate

Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year: 1997
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: The following validity criteria were fulfilled: (1) degradation rate of the reference substance had reached a level of 60% within 14 days, (2) parallel assays did not differ by more than 20%, (3) CO2 evolution in the inoculum blank did not exceed 40 mg/l at the end of the test, (4) IC content of the test substance suspension in mineral medium at the start of the test was less than 5% of the total carbon.

Result: Kinetic of control substance: 6 days = 40%

16 days = 102%
28 days = 105%

The test substance attained 62% degradation over the test period. However, the 60% pass level was not reached within the 10 day window, therefore it cannot be considered readily biodegradable.

Test condition: Concentration of activated sludge: 30 mg dry matter/l
Test volume: 3 L
Temperature: 21°C
pH: not reported

Reliability: (1) valid without restriction

Flag: Critical study for SIDS endpoint

Reference: Mead, C. 1997c. Kalcohl 6098: Assessment of readily biodegradability; CO2 evolution test. SPL Project Number 140/543.

17-OCT-2005 (59)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: aerobic

Inoculum: other: activated sludge, predominantly domestic

Concentration: 100 mg/l related to COD (Chemical Oxygen Demand)

Contact time: 28 day(s)

Degradation: = 76 % after 28 day(s)

Result: inherently biodegradable

Kinetic: 7 day(s) = 40 %
14 day(s) = 59 %
21 day(s) = 67 %
28 day(s) = 76 %

Control Subst.: other: Sodium acetate

Method: other: ISO 10708 (BODIS) and RDA Blok Test

Year: 1992

GLP: yes

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: The test method used is based on OECD test method 301D and the RDA-Blok-Test. Mineral medium was inoculated with activated sludge and stabilized for one week at 20-25 C with continuous stirring. After stabilisation, 200 ml of test medium was filled into 300 ml bottles, aerated until O2 saturation was reached and spiked with test substance by directly weighing into the test vessels. Vessels were filled 2/3, stoppered and shaken continuously at 20-25 degree C.
Degradation was followed by weekly measurements of BOD using an O2-electrode. Oxygen consumption resulting from biodegradation of the test substance was corrected by oxygen

uptake of blank inoculum. Degradation rate was calculated as % BOD/COD.

Remark: The validity criteria were fulfilled: (1) degradation rate of the reference substance had reached a level of 60% within 14 days, (2) total oxygen uptake in blanks after the first week was lower than 3 mg O2 and lower then 1 mg O2 in the following weeks, (3) residual concentration of O2 in test bottles did not fall below 0.5 mg/l.
However, the parallel assays did not fall within the acceptable 20% range. On day 28, the % degradation for the three replicates was 71%, 91% and 67%.

Result: Kinetic of control substance:
7 days = 81%
14 days = 95%
21 days = 97%
28 days = 98%
The test substance attained 76% degradation over the test period. However, the 60% pass level was not reached within the 10 day window, therefore it cannot be considered readily biodegradable. However, significant degradation was observed therefore the substance is considered to be inherently biodegradable.

Test condition: Concentration of activated sludge: 30 mg dry matter/l
Test volume: 200 ml
Temperature: 20-25 C
pH: not reported

Reliability: (2) valid with restrictions
The test failed to meet one of the validity criteria of the test guideline.

Reference: Henkel KGaA. 1992a. Lorol C16-98: Bewertung der biologischen Abbaubarkeit im BODIS-Test (Aerobic biodegradation: BODIS test/ Two-phase closed bottle test). Biological Research and Product Safety/Ecology: Report No. RE 920102; test substance registration No. SAT 910721, test run No. 120. 26 Juni 1992.

17-OCT-2005 (42)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)</u>

Type: aerobic
Inoculum: other: no information provided on inoculum
Concentration: 20 mg/l related to Test substance
Contact time: 31 day(s)
Degradation: = 61 % after 31 day(s)
Result: inherently biodegradable
Kinetic: 4 day(s) = 27 %

10 day(s) = 47 %
17 day(s) = 59 %
24 day(s) = 60 %
31 day(s) = 61 %

Control Subst.: other: Sodium benzoate

Method: other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
Year: 1994
GLP: no data
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 301B Modified Sturm Test) with one exception: after the samples were added, dichloromethane (30 ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the solvent was evaporated leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
Remark: There is no information given on the validity criteria.
Result: Kinetic of control substance:
4 days = 47.1%
10 days = 58.1%
17 days = 60.5%
24 days = 61.2%
31 days = 62.2%
The test substance attained <60% degradation over the test period therefore it cannot be considered readily biodegradable.
Reliability: (4) not assignable
The information reported is insufficient to assess the validity of this study.
Reference: Vista Chemical Company. 1994. Biodegradability of eleven VISTA ALFOL alcohols. TSR No. 6940-10-05-94.
17-OCT-2005 (96)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)</u>

Type: anaerobic
Inoculum: other: activated sludge from municipal sewage digester
Concentration: 10 mg/l related to test substance
Contact time: 28 day(s)
Degradation: = 97 % after 28 day(s)

Method: other

Year: 1985
GLP: no data
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: Model sludge digester utilizing 14C-radio-labelled test compound and conducted at mesophilic temperatures (35 degree C)
Remark: The publication describes in detail the test system and method used to evaluate the anaerobic biodegradability of several materials including 14C-cetyl alcohol obtained from Amersham-Buchler in Germany.
Result: Total gas production for the fatty alcohol was 97.1% (25.1% as 14CH4 and 72% as 14CO2). Approximately 4% of the starting material remained in the sludge and approximately 0.5% was in the supernatant.
Test condition: Concentration of inoculum: 45 g of centrifuged activated sludge (corresponding to 3 g of dry sludge)
Test volume: 300 ml
Temperature: 35 C
pH: Adjusted to 7 at start of test
Reliability: (2) valid with restrictions
Well-documented scientific study.
Reference: Steber, J. and Wierich, P. 1987. The anaerobic degradation of detergent range fatty alcohol ethoxylates. Studies with 14C-labeled model surfactants. Water Research. 21:6, 661-667.
30-AUG-2005 (84)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: anaerobic
Inoculum: other: municipal sewage digester sludge fortified with activated sludge
Concentration: 1 mg/l related to test substance
Contact time: 28 day(s)
Degradation: = 90.1 % after 28 day(s)

Method: other
Year: 1996
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: Batch test system using C14-labelled material modified after Steber and Wierich 1987
Remark: The method involves a batch test system with a domestic wastewater treatment sludge inoculum. The evolution of radiolabeled carbon dioxide and methane are monitored. The test temperature is 35 degrees C. Starting solids levels of

the test sludge ranged between 24 and 29 g/L.
C14-hexadecanol (labeled in the first carbon) was obtained from Sigma Chemical in St. Louis, MO (purity >98%) and hexadecanol was obtained from American Tokyo Kasei Inc. in Portland, OR. The final ratio of C14 -CO2 to C14 -CH4 in the gas produced was 3.3 to 1. The mechanism of hexadecanol biodegradation would be catabolized by beta oxidation to form acetate. Hexadecanol degradation exhibited first-order kinetics.

Result: Total gas production for hexadecanol was 90.1% (69.1% as 14CO2 and 21.0% as 14CH4). Approximately 9% of the starting material remained with the solids and 0.5% remained in solution.

Reliability: (2) valid with restrictions
Well-documented scientific study.

Reference: Nuck, B.A. and Federle, T.W. 1996. Batch test for assessing the mineralization of 14C-radiolabeled compounds under realistic anaerobic conditions. Environ. Sci. Technol. 30:12, 3597-3603.

30-AUG-2005 (65)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: aerobic
Inoculum: predominantly domestic sewage
Concentration: .05 mg/l related to test substance
Degradation: = after 5 day(s)

Test substance: >= 95% 1-hexadecanol (36653-82-4)
Remark: Messgroessen: Konzentration der Testsubstanz, CO2-Entwicklung radioaktiv markierte Testsubstanz.
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: 25 Grad C; Ansatz geruehrt
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

Reference: Freitag, D. et al., Ecotoxicol. Environ. Saf. 6, 60-81 (1982).

09-JAN-2005 (26)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: aerobic

Inoculum: predominantly domestic sewage
Concentration: 50 µg/l related to test substance
Degradation: = 28 % after 5 day(s)

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Messgroesse: 14CO2-Entwicklung
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: U-14C Hexadecanol; Ruehren; T = 24-26 Grad C
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Freitag, D. et al., Chemosphere 14, 1589-1616 (1985).
09-JAN-2005 (24)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: aerobic
Inoculum: predominantly domestic sewage
Concentration: 50 µg/l related to test substance
Degradation: = 37 % after 5 day(s)

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Messgroesse: 14CO2-Entwicklung
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: U-14C Hexadecanol; Ruehren; T = 24-26 Grad C
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Freitag, D. et al., Ecotox. Environ. Safety 3, 144-151 (1979).
09-JAN-2005 (25)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: aerobic
Inoculum: other bacteria: Marines Sediment (adaptiert)
Concentration: 1.7 mmol/l related to Test substance
Degradation: = 96 % after 42 day(s)

Kinetic: 25 day(s) = 62 %

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Messgroesse: substanzspezifische Analytik (IR-Spektroskopie)
Werte aus graphischer Darstellung entnommen
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: T = 16 Grad C; Schuetteln
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Hoepner, T. et al., Ecol. Stud. 73, 251-271 (1989).
09-JAN-2005 (46)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: anaerobic
Inoculum: other bacteria: Marines Sediment (adaptiert)
Concentration: 1.7 mmol/l related to test substance
Degradation: = 90 % after 121 day(s)
Kinetic: 63 day(s) = 67 %

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Messgroesse: substanzspezifische Analytik (IR-Spektroskopie)
Werte aus graphischer Darstellung entnommen
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: T = 16 Grad C; Schuetteln
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Hoepner, T. et al., Ecol. Stud. 73, 251-271 (1989).
09-JAN-2005 (46)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Type: anaerobic
Inoculum: other bacteria: Mischung aus Belebtschlamm und Faulschlamm
Concentration: 10 mg/l related to Test substance
Degradation: = 97.1 % after 28 day(s)

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Messgroesse: Gasentwicklung (14CO2 & 14CH4)
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: 35 Grad C; radioaktiv markierte Testsubstanz; periodisches Umruehren des Testansatzes (alle 12 h)
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Steber, J. & Wierich, P., Water Res. 21, 661-667 (1987).
09-JAN-2005 (83)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Degradation: = 0 % after 5 day(s)

Method: other: BSB-Bestimmung nach AFNOR-Richtlinie NF T90/103 (1969)
Year: 1969
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Abbaugrad: 0 % (Sauerstoffmangel durch Bildung eines Oberflaechenfilms?)
Einsatzkonzentration: nicht angegeben
Inokulum: nicht angegeben
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Dore, M. et al., La tribune de cebedeau 28, 3-11 (1975).
09-JAN-2005 (20)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Inoculum: activated sludge, non-adapted
Concentration: 500 mg/l related to Test substance
Degradation: = 0 % after 1 day(s)

Method: other: Warburg-Respirometer
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Abbauversuche mit drei Belebtschlaemmen unterschiedlicher Herkunft
der Stoff wirkte auf jeden der getesteten Belebtschlaemme toxisch (Sauerstoffmangel durch Bildung eines Oberflaechenfilms?)
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: 20 Grad C
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Gerhold, R. and Malaney, G. (1966). Structural determinants in the oxidation of aliphatic compounds by activated sludge. J. Water Poll. Control Fed. 38:562-579.
09-JAN-2005 (29)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Inoculum: predominantly domestic sewage
Concentration: 73 mg/l related to test substance
Degradation: = 14.3 % after 20 day(s)

Test substance: >= 95% 1-hexadecanol (36653-82-4)
Remark: durchgehender Oberflaechenfilm (begrenzte Bioverfuegbarkeit)
Messparameter: Gewichtsverlust des eingesetzten Hexadecanols nach Methanolextraktion
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: T = 20 Grad C; schwache Belueftung
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Ludzack, F.J. & Ettinger, M.B., J. AWWA 49, 849-858 (1957).
09-JAN-2005 (56)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Inoculum: predominantly domestic sewage, adapted
Concentration: 76 mg/l related to test substance
Degradation: = 8.6 % after 37 day(s)

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: durchgehender Oberflaechenfilm (begrenzte Bioverfuegbarkeit) Messparameter: Gewichtsverlust des eingesetzten Hexadecanols nach Methanolextraktion
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: T = 20 Grad C; schwache Belueftung
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Ludzack, F.J. & Ettinger, M.B., J. AWWA 49, 849-858 (1957)
09-JAN-2005 (56)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Inoculum: other bacteria: Pseudomonas sp. (adaptiert)
Concentration: 800 µmol/l related to test substance
Degradation: ca. 66 % after 2 day(s)

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Alkohole (C10 - C18) als Gemisch geprueft; Einzel-Abbauraten aus GC-Peaks bestimmt; Abbau-Werte aus Graphik ermittelt
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: Inkubation in Minimalmedium mit Gemisch aus Alkoholen (C10, C12, C14, C16 & C18) in Konzentrationen zu je 0.8 mmol/l; geschuettelt; T = 30 Grad C
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: Williams, J. P. et al., Appl. Microbiol. 14, 156-160 (1966).
09-JAN-2005 (102)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Method: Laboratory continuous activated sludge study.

4 mg/L of TS
20ºC
Hydraulic residence time (HRT) 6 h
Sludge retention time (SRT) 10 d

The feed to the sludge unit was of sterile synthetic sewage and AE concentrate and non-sterile tap water.

19 d acclimation was used, followed by 10 days of evaluation. At the start the unit was seeded with sewage treatment plant (STP) activated sludge.

The unit was sampled several times per week, and the samples were analysed immediately.

Analytical recovery of the alcohols was high.

The results showed that the CAS unit was running in a similar way to a full scale STP.

Remark: This paper describes mainly the properties of alcohol ethoxylates (AE) but contains valuable data about the properties and environmental exposures of alcohols themselves. This study should not be considered as a study of alcohols alone, but is important in that it indicates that the extent of removal of alcohols from an exposure route that can be anticipated. This extent is high. The waste water organisms were exposed principally to ethoxylates, but the alcohols would be generated by the degradation of the ethoxylates.

Result: Results are corrected for control values.

Alcohol	Conc. in effluent ng/L	Conc. in sludge µg/g	%removal
C12	18	0.6	98.6
C13	21	0.7	99.5
C14	5.5	0	99.6
C15	2.9	1.1	99.8
C16	1.6	0.01	99.5
C18	58	0.7	99.1
Total	130	2	99.4

Total elimination of ethoxylates 97.4
Total in waste sludge solids 2.0
Total in suspended solids 0
This shows that most of that which does not degrade (itself a small amount) is in the solids.

Test substance: 2:1 mixture of NEODOL 25-7 and GENAPOL T110

Alkyl chain distribution

C	Mol ratio
12	1
13	2
14	2.3

15 1.8
16 1.1
18 2.9

Reliability: (2) valid with restrictions
OECD 303. Public domain paper based on a fuller Shell laboratory report.

Reference: T. Wind, R.J. Stephenson, C.V. Eadsforth, A. Sherren, R. Toy. Ecotox and Environ Safety, in press. Determination of the fate of alcohol ethoxylate homologues in a laboratory continuous activated sludge unit.

21-DEC-2005 (86)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Method: The study was a batch-mode activated sludge die-away system. Two treatments consisting of 1 litre each of biologically active sludge were prepared for each test substance. The 14-C alcohols were dissolved in methanol, which was diluted in water and dosed into the sludge in 2-litre flasks.

Disappearance of parent, formation and disappearance of metabolites, uptake into biomass and mineralization to 14-C CO2 were monitored over time.

Activated sludge from a municipal WWTP was obtained, and used at 2500 mg/L.

The TS was dosed at 0.05 µM: this is equivalent to 9.3µg/L (C12), 10.0 µg/L (C14), 10.7 µg/L (C16); added to flasks at 20ºC.

Remark: The results for three substances are considered alongside each other since the results of the whole study are useful to show the consistency of the results.

Result: Recoveries were high.

After 48h incubation:

C	Parent	metabolites	Water	Solids	CO2
C12	0.8	5.9	3.5	20.7	73.9
C14	1.3	6.3	2.0	21.0	76.7
C16	2.6	11.5	2.1	17.0	65.3

Concentrations were modelled with the equation
C = Ae^(-k1t) + B(e^-k2t)
(a two compartment first order decay model)

%	A	k1 h-1	B	k2 h-1
C12	82±2	113±8	9±1	0.36±0.1
C14	82±2	87±5	12±1	0.30±0.1
C16	41±3	103±23	48±2	0.43±0.04

The results show the high biodegradability of C12 to 16 alcohols in activated sludge.

Test substance: Radiolabelled (14C) C12, C14 and C16 alcohols.

Reliability: (2) valid with restrictions
Non-standard study conducted to a scientifically sound method.

Reference: T.W. Federle, N.R. Itrich, 'Fate of Free and linear alcohol-ethoxylate-derived fatty alcohols in activated sludge'. Ecotox. Environ. Safety, in press.

21-DEC-2005 (87)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (19141-82-3)

Method: Effluent monitoring of waste water treatment plants receiving predominantly municipal effluent. Concentration of alcohols and alcohol ethoxylates were measured.

Twenty-four hour composite samples of influent and effluent were collected from each of the locations from three days. They were preserved with formalin at the time of collection. These were composited in proportion to flow.

Samples of 4 litres ware obtained and extracted onto a succession of cartridges, followed by solvent elution. Quantitative analysis of the eluates was by a derivitisation Liquid-chromatography-mass spectrometric (LCMS) technique.

Result: Influent (In), effluent (Eff) values in ug/l, and % removal of alcohols are indicated in the table below, with alcohol data considered in two groups. The State in which the WWTP is found is indicated by the usual 2-letter abbreviation.

	C12-15 OH			C16-18 OH		
WWTP type	In	eff	%	in	eff	%
TX Lagoon	297	2	99.3	92.7	2.4	97.4
NJ Oxidation Ditch	249	0.7	99.7	181	0.8	99.6
OH Rotating biological contactor	157	0.1	0.06	77	0.07	99.9

IA	Trickling filter	499	2.0	99.6	354	2.3	99.4
MO	Trickling filter	532	4.9	99.1	315	9	97.3
KS	Lagoon	67.5	1.1	98.4	35.4	2.2	93.8
CA	Activated sludge	20.05	0.2	99.9	169	0.4	99.8
OR	Activated sludge	92.9	0.2	99.8	133	0.6	99.5
AZ	Oxidation ditch	702	0.3	100	394	0.5	99.9

Results for the carbon number groups are considered alongside each other to enable the context of every data point to be seen. In the overall interpretation of the data, the results have been used with those from other studies to determine the contribution of measured alcohol concentrations from various sources.

Reliability: (2) valid with restrictions
Non-GLP studies conducted to a high standard.

Reference: S.W. Morrall, J.C. Dunphy, M.L. Cano, A. Evans, D.C. McAvoy, B.P. Price, W.S. Eckhoff. 'Removal and environmental exposure of alcohol ethoxylates in US sewage treatment', Ecotox. Environ. Safety, in press.

21-DEC-2005 (72)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)

Type: aerobic
Inoculum: other: effluent from a domestic sewage treatment plant
Concentration: 2 mg/l related to test substance
5 mg/l related to test substance
Contact time: 29 day(s)
Degradation: = 69 - 38 % after 29 day(s)
Result: inherently biodegradable

Method: other: EEC Directive 92/69/EEC, C.4-E
Year: 1992
GLP: no data
Test substance: Octadecanol (112-92-5)

Method: This test method corresponds to OECD 301D.

Remark: Due to the low water solubility of the test substance, a homogenous distribution was achieved by ultrasound dispersion and stabilization by an inert emulsifier. The dispersing agent was nonylphenol ethoxylate additionally propoxylated with 5 propyleneoxide units (NP 9,5 EO 5PO). The following validity criteria were met: (1) the parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level within 14 days, (3) oxygen depletion in the inoculum blank did not exceed 1.5 mg/l after 30 days, and (4) the residual concentration of oxygen in the test bottle did not fall below 0.5 mg/l.

Result: 7 days = 30 - 17%
14 days = 52 - 21%
21 days = 59 - 34%
28 days = 69 - 38%
Two concentrations of test material were tested: 2 mg/l and 5 mg/l. In the results section, the first values cited are for the 2 mg/l concentration and the second are for the 5 mg/l concentration.
The final result was greater than the 60% BOD/ThOD threshold but it did not reach this level within the 14 day window which is the criterion for classification of "ready biodegradability." At a test concentration of 5 mg/L the BOD/ThOD reached only 38% at 28 days. The reference substance, Sodium benzoate degraded by 88% after 29 days.

Source: Henkel KGaA 1992f.

Test condition: Inoculum concentration: 1 ml/l
Test volume: not reported
Temperature: 20 C
pH: not reported

Reliability: (1) valid without restriction

Flag: Critical study for SIDS endpoint

Reference: Henkel KGaA. 1992f. Lorol C18-98: Bewertung der biologischen Abbaubarkeit in GF-Test [Aerobic biodegradation, closed bottle test]. Report No. RE920246, 18 December 1992.

29-OCT-2003 (7)

<u>1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)</u>

Type: aerobic

Inoculum: activated sludge

Concentration: 100 mg/l related to COD (Chemical Oxygen Demand)

Contact time: 28 day(s)

Degradation: = 67 % after 28 day(s)

Result: inherently biodegradable

Method: other: ISO 10708 (BODIS)
Year: 1992
GLP: no data
Test substance: Octadecanol (112-92-5)

Method: The test method used is based on OECD test method 301D and the RDA-Blok-Test. It is especially suitable for poorly water-soluble compounds. The test medium is inoculated and the test chemical added. The test vessels are then closed and shaken continuously. Weekly measurements of the BOD from the aqueous phase are taken.
Remark: The following validity criteria were met: (1) the parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level within 14 days, (3) the residual concentration of oxygen in the test bottle did not fall below 0.5 mg/l.
It could not be determined whether O2 depletion in the blank surpassed 1.5 mg/l after 28 days as no data was provided on Day 0 O2 concentrations.
Result: 7 days = 25%
14 days = 52%
21 days = 66%
28 days = 67%
The substance degraded <60% in the 14 day window. It took 20 days to degrade 60%. The reference substance, Sodium acetate, degraded by 86% after 28 days.
Source: Henkel KGaA 1992g.
Reliability: (1) valid without restriction
Not key study: Other studies (same reliability score) but with higher degradation rate are available.
Reference: Henkel KGaA. 1992g. Lorol C18-98: Bewertung der biologischen Abbaubarkeit im BODIS-Test. Report No. RE 920028. 5 March 1992.
29-OCT-2003 (8)

<u>1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)</u>

Type: aerobic
Inoculum: other: no information on inoculum
Concentration: 20 mg/l related to Test substance
Contact time: 31 day(s)
Degradation: = 67 % after 31 day(s)
Result: inherently biodegradable

Method: other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation

Test
Year: 1994
GLP: no data
Test substance: Octadecanol (112-92-5)

Method: This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 301B Modified Sturm Test) with one exception: after the samples were added, dichloromethane (30ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the solvent was evaporated leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
Remark: There is no information given on the validity criteria.
Result: 4 days = 30%
10 days = 52%
17 days = 65%
24 days = 67%
31 days = 67%
The test substance attained <60% degradation during the 10 day window. Sodium benzoate was used as a positive control and reached a mineralization extent of 62.2%.
Source: Vista 1994.
Test substance: The substance corresponds to CAS# 112-92-5. Tradename is ALFOL 18.
Reliability: (2) valid with restrictions
Not key study: Other studies with higher reliability score and higher degradation rates are available.
Reference: Vista Chemical Company. 1994. Biodegradability of eleven VISTA ALFOL alcohols. TSR No. 6940-10-05-94.
31-OCT-2003 (15)

<u>1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3985-81-7)</u>

Type: aerobic
Inoculum: activated sludge, domestic
Concentration: 20 mg/l related to COD (Chemical Oxygen Demand)
Contact time: 28 day(s)
Degradation: = 43 % after 28 day(s)
Result: inherently biodegradable

Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year: 1997
GLP: yes
Test substance: Octadecanol (112-92-5)

Method: The test material was exposed to activated sewage sludge micro-organisms at a concentration of 20 mg C/l with culture medium in sealed culture vessels in the dark at 21 degree C for 28 days. The degradation of the test material was assessed by the determination of carbon dioxide produced. Control solutions with inoculum and the standard material, sodium benzoate were used for validation purposes.

Remark: The following validity criteria were met: (1) the parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level within 14 days, (3) total CO2 evolution in the inoculum blank did not exceed 40 mg/l at the end of the test and (4) IC content of the test substance suspension in mineral medium at the start of the test was less than 5% of the total carbon.

Result: 8 days = 10%
14 days = 35%
20 days = 39%
28 days = 43%
The test material attained 43% degradation after 28 days and therefore cannot be regarded as readily biodegradable. The reference substance Sodium benzoate, attained 105% degradation after 28 days.

Source: Mead 1997d.

Test substance: This substance corresponds to CAS# 112-92-5. Tradename is Kalcol 8098.

Reliability: (1) valid without restriction
Not key study: Other studies (same reliability score) but with higher degradation rate are available.

Reference: Mead, C. 1997d. Kalcohl 8098: Assessment of readily biodegradability; CO2 evolution test. SPL Project Number 140/544.

10-SEP-2003 (11)

<u>1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)</u>

Result: inherently biodegradable

Method: other: read-across based on grouping of substances (category approach)

Year: 2005

GLP: no

Test substance: >= 90% 1-eicosanol (629-96-9)

Remark: This substance is predicted to be inherently biodegradable. This conclusion is drawn from analysis of trends in results

measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance is not expected to affect the rate of biodegradability.

Reliability: (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

Flag: Critical study for SIDS endpoint

Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

21-DEC-2005 (3)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Type: aerobic
Inoculum: activated sludge, domestic
Concentration: 12.4 mg/l related to Test substance
Contact time: 28 day(s)
Degradation: = 37 % after 28 day(s)
Result: other: not readily biodegradable
Kinetic: 8 day(s) = 16 %
10 day(s) = 23 %
14 day(s) = 29 %
22 day(s) = 33 %
28 day(s) = 37 %
Control Subst.: other: Sodium benzoate

Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year: 2000
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)

Method: The test material was exposed to activated sewage sludge micro-organisms at a concentration of 10 mg C/l with culture medium in sealed culture vessels in the dark at 21 C for 28 days.

The degradation of the test material was assessed by the determination of carbon dioxide produced. Control solutions with inoculum and the standard material, sodium benzoate, together with a toxicity control were used for validation

purposes.

Remark: The following validity criteria were met:
(1) The IC/TC ratio of the test material suspension in the mineral medium at the start of the test was below 5%,
(2) the total CO2 evolution in the control vessels on day 28 was 37.85 mg/l (= 113.55 mg/3 l),
(3) degradation of reference substance reached pass level within 14 days,
(4) toxicity control (KALCOL 220-80 and sodium benzoate) degraded by 42% after 14 days, and
(5) results of parallel assay did not differ from each other by more than 20%.

Result: Kinetic of control substance:
8 days = 59%
10 days = 63%
14 days = 64%
22 days = 64%
28 days = 74%
The test material degraded <60% over the test period therefore it cannot be considered readily biodegradable.

Test condition: Concentration of inoculum: 30 mg suspended solids (ss)/l
Test volume: 3000 ml
Temperature: 21 C
pH: not reported

Reliability: (1) valid without restriction

Flag: Critical study for SIDS endpoint

Reference: Mead, C. 2000. Kolcol 220-80: Assessment of ready biodegradability; CO2 evolution test. Safepharm Laboratories, SPL Project Number 140/1002.

17-OCT-2005 (22)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-2)</u>

Method other: modeled data

Remark BIOWIN v4.02 Results - predictions:

Linear Model: Biodegrades Fast
Non-Linear Model: Biodegrades Fast
Ultimate Biodegradation Timeframe: Weeks
Primary Biodegradation Timeframe: Days-Weeks
MITI Linear Model: Biodegrades Fast
MITI Non-Linear Model: Biodegrades Fast

Reliability (4) not assignable

Reference BIOWIN v4.02. US EPA, 2006.

04-APR-07

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Method other: modeled data

Remark BIOWIN v4.02 Results - predictions:

Linear Model: Biodegrades Fast
Non-Linear Model: Biodegrades Fast
Ultimate Biodegradation Timeframe: Weeks
Primary Biodegradation Timeframe: Days-Weeks
MITI Linear Model: Biodegrades Fast
MITI Non-Linear Model: Biodegrades Fast

Reliability (4) not assignable
Reference BIOWIN v4.02. US EPA, 2006.
04-APR-07

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Method other: modeled data

Remark BIOWIN v4.02 Results - predictions:

Linear Model: Biodegrades Fast
Non-Linear Model: Biodegrades Fast
Ultimate Biodegradation Timeframe: Weeks-Months
Primary Biodegradation Timeframe: Days-Weeks
MITI Linear Model: Biodegrades Fast
MITI Non-Linear Model: Biodegrades Fast

Reliability (4) not assignable
Reference BIOWIN v4.02. US EPA, 2006.
04-APR-07

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Method other: modeled data

Remark BIOWIN v4.02 Results - predictions:

Linear Model: Biodegrades Fast
Non-Linear Model: Does Not Biodegrade Fast
Ultimate Biodegradation Timeframe: Weeks-Months
Primary Biodegradation Timeframe: Days-Weeks
MITI Linear Model: Biodegrades Fast
MITI Non-Linear Model: Biodegrades Fast

Reliability (4) not assignable

Reference BIOWIN v4.02. US EPA, 2006.
04-APR-07

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Water 3.7 Bioaccumulation

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Elimination	
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Not expected to bioconcentrate.
Reliability	(4) not assignable
Reference	HSDB (2003) Hazardous Substances Databank. US National Library for Medicine.
19.10.2004	(5)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

BCF	3.16
Elimination	
Method	other: modeled
Year	
GLP	
Test substance	ethanol (64-17-5)
Remark	Bcfwin v2.15
	Log Kow (estimated) : -0.14 Log Kow (experimental): -0.31 Log Kow used by BCF estimates: -0.31
	Equation Used to Make BCF estimate: Log BCF = 0.50
	Correction(s): Value Correction Factors Not Used for Log Kow < 1
	Estimated Log BCF = 0.500
Reliability	(4) not assignable
Reference	U.S. EPA URL http://www.epa.gov/opptintr/exposure/docs/episuite.htm
19.10.2004	(64)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Type:	Bioconcentration Factor (BCF)
Test substance:	1-butanol (CAS No. 71-36-3)

Method: Calculated using EPISUITE v.3.IO and BCFWIN v.2.14 with a log Kow of 0.88.
Result: 3.162 L/kg
GLP: Not applicable
Reliability: (2) valid with restrictions, calculated value
Reference: EPISUITE v.3.10, U.S. Environmental Protection Agency, April (2001).

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

BCF: = 11

Method: other: calculated (Veith et al, 1979)
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Method: For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 2.03 was used in the calculation.
Remark: Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method.
Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.
21-DEC-2005 (3)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

BCF: = 95

Method: other: calculated (Veith et al, 1979)
Year: 2004
GLP: no

Test substance: > 90% 1-octanol (111-87-5)

Method: For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 3.15 was used in the calculation

Remark: Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method.

Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

21-DEC-2005 (5)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

BCF: = 1530

Method: other: calculated (Veith et al, 1979)
Year: 2004
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Method: For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 4.57 was used in the calculation.

Remark: Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method.

Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

21-DEC-2005 (4)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)

BCF: = 3801

Test substance: other TS: Dodecanol (112-53-8)

Remark: The modeled result reported in the 1993 Dossier is considerably higher than the modeled result using the EPISuite model in 2000.

Source: SIDS Dossier 1993a.

Reliability: (2) valid with restrictions

Reference: SIDS Dossier on 1-Dodecanol. 1993a. Environmental Protection Agency, Denmark. 6 June 1993.

25-SEP-2003 (19)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

BCF: = 33900

Method: other: calculated (recalculated from Connell and Hawker, 1988)

Year: 2004

GLP: no

Test substance: > 95% 1-Tetradecanol (112-72-1)

Method: For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 6.03 was used in the calculation.

Remark: Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method.

Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

21-DEC-2005 (5)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Species: other: activated sludge

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Bioakkumulationsfaktor:
Belebtschlamm: 1300 (5 d; T = 24-26 Grad C; Ruehren; aerob experimentell bestimmt mit 50 ug/l U-14C Hexadecanol, keine substanzspezifische Analytik, nur Radioaktivitaet gemessen (14C-Einbau in Biomasse).

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

Reference: Freitag, D. et al., Ecotox. Environ. Safety 3, 144-151 (1979).

09-JAN-2005 (25)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Species: other: see remarks

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Bioakkumulationsfaktoren:
Chlorella fusca (Alge): 17 000 (24 h; T=20-25 Grad C; Schuetteln)
Belebtschlamm: 3170 (5 d; T = 24-26 Grad C; Ruehren; aerob)
Leuciscus idus melanotus (Goldorfe): 56 (3 d; T = 20-25 Grad C; Ruehren;
keine Fuetterung).
50 ug/l U-14C Hexadecanol; keine substanzspezifische

Analytik, nur Radioaktivitaet gemessen (14C-Einbau in Biomasse).

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

Reliability: (4) not assignable

This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

Reference: Freitag, D. et al., Chemosphere 14, 1589-1616 (1985)

Freitag, D. et al., Ecotoxicol. Environ. Saf. 6, 60-81 (1982)

Geyer, H et al., Chemosphere 10, 1307-1313 (1981).

09-JAN-2005 (24) (26) (32)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

BCF: = 45300

Method: other: calculated (recalculated from Connell and Hawker, 1988)

Year: 2004

GLP: no

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 6.65 was used in the calculation

Remark: Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

Reliability: (2) valid with restrictions

The value was predicted using an accepted calculation method.

Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

21-DEC-2005 (5)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

BCF: = 100000

Test substance: other TS: Octadecanol (112-92-5)

Remark: The modeled estimate reported in the 1993 Dossier is considerably higher than the modeled estimate using the EPISuite model in 2000.
Source: SIDS Dossier 1993b.
Reliability: (2) valid with restrictions
Reference: SIDS Dossier on 1-Octadecanol. 1993b. Environmental Protection Agency, Denmark. 6 June 1993.
25-SEP-2003 (12)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

BCF: = 31800

Method: other: calculated (recalculated from Connell and Hawker, 1988)
Year: 2004
GLP: no
Test substance: 1-eicosanol (629-96-9)

Method: For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 7.75 was used in the calculation.
Remark: Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method.
Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

21-DEC-2005 (3)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

BCF: = 31800

Method: other: calculated (recalculated from Connell and Hawker, 1988)
Year: 2004
GLP: no
Test substance: 1-docosanol (661-19-8)

Method: For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The estimated log Kow value of 7.75 was used in the calculation.

Remark: Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method.

Reference: Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

21-DEC-2005 (3)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

BCF: = 3.162

Method: other: calculated (recalculated from Connell and Hawker, 1988)
Year: 2006
GLP: no
Test substance: 1-tetracosanol

Method: For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation

was used. This approach is in accordance with standard EU recommendations. For substance with log Kow > 7 a minimum log BCF of 0.50 was used.

The estimated log Kow value of 10.66 was used in the calculation.

Remark: Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method.

Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.
05-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

BCF: = 3.162

Method: other: calculated (recalculated from Connell and Hawker, 1988)
Year: 2006
GLP: no
Test substance: 1-hexacosanol

Method: For substances with log Kow <6, the Veith et al. linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations. For substance with log Kow > 7 a minimum log BCF of 0.50 was used.
The estimated log Kow value of 11.65 was used in the calculation.

Remark: Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.
The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method.

Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.

05-APR-2007

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

BCF: = 3.162

Method: other: calculated (recalculated from Connell and Hawker, 1988)
Year: 2006
GLP: no
Test substance: 1-octacosanol

Method: For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations. For substance with log Kow > 7 a minimum log BCF of 0.50 was used.
The estimated log Kow value of 12.63 was used in the calculation.
Remark: Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.
Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method.
Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.
05-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

BCF: = 3.162

Method: other: calculated (recalculated from Connell and Hawker, 1988)
Year: 2006
GLP: no
Test substance: 1-triacontanol

Method: For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations. For substance with log Kow > 7 a minimum

log BCF of 0.50 was used.

The estimated log Kow value of 13.61 was used in the calculation.

Remark: Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.
The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

Reliability: (2) valid with restrictions
The value was predicted using an accepted calculation method.

Reference: EPISUITE v. 3.12, U.S. Environmental Protection Agency, 2006.

05-APR-2007

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Static
Species	Salmo gairdneri (Fish, estuary, fresh water)
Exposure period	96 hour(s)
Unit	mg/l
LC50	= 13000 measured/nominal
Limit test	
Analytical monitoring	No
Method	other
Year	1978
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Biological observations: None described. Table of cumulative mortality: Not presented. Lowest concentration causing 100% mortality: Not stated. Mortality in controls: Not discussed. Abnormal responses: Not discussed. Reference substance: None used. Any observations (e.g. precipitation) that might cause a difference between measured and nominal values: Not discussed. Oncorhynchus mykiss and Salmo gairdneri are synonyms The Columbia National Fisheries Research Laboratory conducted

aquatic toxicity tests on more than 400 chemicals during 1965-1978; this is a major research area for the lab.
The lab. also participated in the development of standard acute toxicity test methodology and only tests meeting acceptable procedures were included in this compilation.

Test organism: Age fingerlings, Length not stated. Weight 0.8g.
Loading <=0.8 g/l fish/litre.
Pretreatment: Acclimated for 1-3 day.
Dilution water source: Reconstituted deionized water.
Dilution water chemistry: hardness 40-50 mg/l CaCO3; Alkalinity 30-35 mg/l CaCO3; pH 7.2-7.5.
Stock solution preparation: Not described.
Flow-through state: Static.
Vehicle, solvent and concentration: Not applicable Solubility: Not applicable.
Exposure vessel type: 18.9 I wide-mouthed jars containing 15 I test solution, not aerated.
Illumination: not stated.
Replicates: 10 fish per concentration; no. of replicates not stated.
Water chemistry on test: Not described.
Test temperature range: 12 deg C +/- 1 deg C.
Method of calculating mean measured concentration: Only nominal concentrations used.

Statistical method: Litchfield and Wilcoxon (1949).

Reliability (2) valid with restrictions Only nominal concentration measurements are available, However, fugacity data suggests low losses would be expected by evaporation. In addition there are no water quality data available and no GLP data.

However, the data is regarded as reliable with restrictions.

Flag Critical study for SIDS endpoint

Reference Johnson, W. and Finley, M. (1980). Handbook of acute toxicity of chemicals to fish and aquatic invertebrates. U.S. Dept of Interior, Fish and Wildlife Service. Washington, DC Resource Publication 137.

17.11.2004 (75)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type flow through
Species Pimephales promelas (Fish, fresh water)
Exposure period 96 hour(s)
Unit mg/l

LC50	= 13480 measured/nominal
Limit test	
Analytical monitoring	No
Method	other
Year	1974
GLP	no data
Test substance	other TS: Reagent grade ethanol (64-17-5)
Method	Ethanol concentrations ranged up to 30,000 mg/l Biological
Remark	observations: Some fish lost equilibrium. Table showing cumulative mortality: Not given. lowest dose causing 100% mortality: Not stated. Mortality of controls: Not discussed. Abnormal response: No abnormal response noted. Reference substances: None. Any other observations affecting concentration: None. These data were collected by the EPA's Environmental research Lab in Duluth, Minnesota, a lab likely to have significant experience in acute toxicity testing of this kind. These data are rated 'probably reliable'. Test organism: Age Juvenile, 4-6 wk; Length 1-3.1 cm; Weight Not stated. Loading: 20 fish/jar in 2 I test water. Pretreatment: Acclimated to flowing water for 48 h. Dilution water source: Lake Superior water. Dilution water chemistry: Not stated. Stock solution preparation: Ethanol weighed in to measured water and whole shaken. Vehicle, solvent and concentration: Not applicable Solubility: Not applicable. Stability: Not measured. Exposure vessel type: Coveredcyclindrical glass battery jars. Illumination: 50 ft-c cool, white fluorescent light 16 h/day. Replicates: 10 fish per concentration, 1 replicate per concentration. Water chemistry on test Not described. DOC kept to 4 mg/l during test. Test temperature range: 18-22 deg C. Method of calculating mean measured concentration: Concentrations not measured.
Result	Statistical method: Standard graphical. This LC50 value was within 50% of values previously reported. LC50 for shorter periods were as follows:

	1 h >18,000 mg/l 24 h >18,000 mg/l 48 h =13,480 mg/l 72 h =13,480 mg/l
Reliability	(2) valid with restrictions
Reference	Mattson, V., Arthur, J. and Wallbridge, C. (1976). Acute toxicity of selected organic compounds to Fathead Minnows. U.S. EPA Environmental Reasearch Lab., Duluth, Minnesota, EPA 600/3-76-097.
12.11.2004	(76)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Static
Species	Pimephales promelas (Fish, fresh water)
Exposure period	4 day(s)
Unit	mg/l
LC50	> 100 measured/nominal
Limit test	Yes
Analytical monitoring	No
Method	other
Year	1986
GLP	no data
Test substance	other TS: Reagent grade ethanol (64-17-5)
Method	Juvenile Pimephales promelas fish (4-8 weeks) were exposed to ethanol for 96 hr. EPA method presumed.
Remark	Biological observations: Not discussed. Minnows were considered dead if they were motionless and failed to respond to prodding. Table showing cumulative mortality: Not given. lowest dose causing 100% mortality: 100% mortality not achieved at any dose. Mortality of controls: Not discussed. Abnormal response: No abnormal response noted. Reference substances: None although several other substances tested. Any other observations: None. Test organism: Age juvenile, not specified; weight 0.2-0.5g. loading: <0.5 wet weightll. Pretreatment: Acclimated; food with-held 24 h. Dilution water source: Activated carbon-filtered, dechlorinated and tempered lake Ontario water. Dilution water chemistry: hardness 130 mg/I CaC03;

	Alkalinity 93 mg/l CaC03, pH 7.4, TOC 1.8 mg/I, TSS 180mg/l; salinity 26 mgll CI Stock solution preparation: Not described. Max concentration tested 100mg/l. Vehicle, solvent and concentration: Not applicable Solubility: Not applicable. Exposure vessel type: Unsealed cubic Pyrex chromatograph dishes. Illumination: 50 ft-c cool, white fluorescent light 16h/day. Replicates: 10 fish per concentration, 1 replicate per concentration. Water chemistry on test: Not described. DOC kept below 40% of starting value. Test temperature range: 20 deg C +1- 0.1 deg C. Method of calculating mean measured concentration: Only nominal concentrations used. Statistical method: Standard graphical.
Result	The 96 hr LC50 was greater than 100 mgll, the maximum concentration tested.
Reliability	(2) valid with restrictions
Reference	Ewell, w., Gorstch, J., Kmge, R. et al. (1986) Simultaneous evaluation of the acute effects of chemicals on seven aquatic species. Environ. Toxicol. Chern. 5:831-840.
17.11.2004	(77)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	Salmo gairdneri (Fish, estuary, fresh water)
Exposure period	1 day(s)
Unit	mg/L
LC50	> 11200 measured/nominal
Limit test	
Analytical monitoring	No
Method	other:
Year	1978
GLP	no data
Test substance	ethanol (64-17-5)
Method	Fish exposed to ethanol at 6 concentrations up to 30,000 mg/I for 24 hr.
Remark	Biological observations: Table of cumulative mortality: Not presented. Lowest concentration causing 100% mortality: in static tests, 25,000 mg/I caused 100% mortality in 3 hr. Mortality in controls: Not discussed.

Abnormal responses: Not discussed.
Reference substance: None used.
Any observations (e.g. precipitation) that might cause a difference between measured and nominal values: None.
Test organism: Age fingerlings, 9.2 cm +/1 1.1 em, weight 9.5 +/- 3.8 g.
Source Caribou Trout ranch, Soda Springs, lhaho Loading 1 fish/litre..
Pretreatment: Acclimated for at least 2 wk.
Dilution water source: Dechlorinated city tap water.
Dilution water chemistry: hardness 90 mg/I CaC03; Conductivity 190 muS/em, pH 8.0.
Stock solution preparation: Not described.
Vehicle, solvent and concentration: Not applicable Solubility: Not applicable.
Exposure vessel type: PET-lined 20 I vessels.
Illumination: 12 h light: 12 h dark cycle.
Replicates: 10 fish per concentration, 1 replicate per concentration.
Water chemistry on test: Not described.
Test temperature range: 10 deg C.
Method of calculating mean measured concentration: Only nominal concentrations used.
Criterion for death: cessation of respiration.

Result
Statistical method: Litchfield (1949 and APHA (1971).
Nominal concentrations achieved: 0.1, 1.0,10 and 100 mgll.
LC50 11,200 mg/I (not achieved).
Reagent grade ethano from Standard Chemicals.

Reliability
(2) valid with restrictions
This was a screening study for a flow through sub-lethal study. Limited results are reported. Design was static with no measured concentrations, however short length of study limits impact of these omissions. Study rated reliable with restrictions.

Reference
Majewski, H., Klaverkamp, J. and Scott, D (1978) Acute mortality and sub-lethal effects of acetone, ethanol and propylene glycol on the cardiovascular and respiratory systems of rainbow trout (Salmo gairdneri) Water Res. 13: 217 - 221.

17.11.2004
(78)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type Other
Species Pimephales promelas (Fish, fresh water)
Exposure period 96 hour(s) g/l
Unit

LC50	= 14.2
EC50	= 14.2
Limit test	
Analytical monitoring	Yes
Method	other: USEPA methodology
Year	1984
GLP	no data
Test substance	ethanol (64-17-5)

Method

Remark

A 96-hour LC50 or 15.3 g/I and a 96-hour EC50 or 12.9 g/I were recorded in an earlier study under the same condition but with 95% ethanol supplied by the U.S. Industrial Chemical Co. Bacterial growth appeared in the exposure tanks. Affected fish were hypoactive and lost equilibrium prior to death.
fathead minnows were cultureds from brood stock provided by the USEPA Environmental Research Laboratory (Duluth). Adults were maintained in flow-through st 25 degC with a 16 -h light/dark photoperiod. Organisms were were fed adult brine shrimp (Artemia). Fry were fed freshly hatched brine shrimp nauplii three times daily until 24-h before test start.
Fish were not fed during exposure to ethanol. 2 replicates of 25 fish were exposed to each of 5 test concentrations and an untreated control in a flow-through system. The tank volume was 6.3 I and the volume additions was 6.46 vol/day.
Test fish were 29-30 day-old at start and had a mean length of 18.2 +/- 2.22 mm and a mean weight of 0.106 +/- 0.036 g.
The loading rate was 0.421 g/I. Reconstituted of filtered Lake Superior water was used for control and dilution water.
Water had hardness of 45 mg/I as CaC03 and an alkalinity of 37.0 mg/I as CaC03.
Nominal (and range of average measured) concentrations (mg/I) tested were 0 (5.4-8.5), 128 (44-48),214 (77-79), 356 (130-137), 594 (235-263) and 990 (398-420). Test temperatures ranged 23.1-25.5 degC. pH ranged 7.3-7.5 SU and dissolved 02 ranged 6.1-7.4 mg/1. Test concentrations in one replicate were measured daily by GLC.
Mortality and adverse effects were reported at 0, 12,21, 24, 48, 52, 72 and 96 hr of exposure and the 96-h EC50/LC50 and 95% confidence limits were estimated using the Trimmed Spearman Karber method.

Test Substance	Test substance was 95% pure ethanol (Aldrich Chemical Co.).
Reliability	(2) valid with restrictions
Reference	Brooke, L.T. et al. (1984) Acute toxicities of organic chemicals to fathead minnows. Vol. 1. University of Wisconsin-Superior.
12.11.2004	(79)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Static
Species	Leuciscus idus melanotus (Fish, fresh water)
Exposure period	48 hour(s)
Unit	mg/l
LC0	= 7110
LC50	= 8140
LC100	= 8690
Limit test	
Analytical monitoring	no data
Method	other
Year	1978
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Method specified in Deutsche Einheitsverfahren zur Wasser-, Abwasser und SchJamm-Untersuchung L 15; Fischtest. Study duration not specified in reference, but authors refer to Mann, H. (1975) Vom Wasser 44, 1 - 3 for details of method. This specifies 48 hours.
Reliability	(4) not assignable
Reference	Juhnke, I. & Luedemann, D. (1978) Ergebnisse der Untersuchung von 200 chemischen Verbindungen auf akute Fischtoxizitaet mit dem Goldorfentest. Z. Wasser Abwasser Forsch. 11. 161 -164.
11.11.2004	(80)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Static
Species	Alburnus alburnus (Fish, estuary)
Exposure period	96 hour(s)
Unit	mg/l
LC50	= 11000
Limit test	
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	
Test Condition	A narcotic effect (loss of equilibrium) was seen in the fishas an early response, followed by coma and then death.

Test Substance	Fish were tested in filtered brackish water (10/tank) at 10 DC in static tanks. At least 6 concentration and one control were tested. Mortality was recorded and the Le50 was determined by probit analysis. The test substance was analytical grade.
Reliability	(4) not assignable
Reference	Bengtsson, B.-E., et al. (1984) Molecular structure and aquatic toxicity - an example with C1 - C13 aliphatic alcohols. Chemosphere 13, 613 - 622. In a similar study, a 96-hour LC50 of 10000 - 11500 mg/l was reported in the bleak (Alburnus alburnus) in a static test at 10 degree C. Linden, E. et al. (1979) The acute. toxicity of 78 chemicals and pesticide formulations against two brackish water organisms, the bleak (Albumus alburnus) and the harpacticoid Nitrocra spinipes. Chemosphere 11/12, 843851.
11.11.2004	(81)(82)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	Semolitus atromaculatus (Fish, fresh water)
Exposure period	24 hour(s)
Unit	mg/l
LC50	= 7000 - 9000 measured/nominal
Limit test	Yes
Analytical monitoring	no data
Method	other
Year	1952
GLP	no data
Test substance	other TS: Commercial grade ethanol (64-17-5)
Remark	This study was to evaluate fish toxicity as a means of determining the critical range of wastewater contamination for 51 different chemicals including ethanol. Critical range is the concentration range (PPM) above which all four fish died in 24 hours and below which all 4 survived over the same period.
Reliability	(4) not assignable
Reference	Gillette, L.A., Miller, D.L., Redman, HE (1952). Appraisal of a chemical waste problem by fish toxicity tests. Sewage Ind. Wastes 24(11):1397-1401.
11.11.2004	(83)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	Oryzias latipes (Fish, fresh water)
Exposure period	15 minute(s)
Unit	mg/l
LC50	= 1000 -10000
Limit test	
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Concentration assumed; endpoint is for physiology; EC50 value assumed. Other fish in same battery of tests were Girella punctata, Chasmichthys dolichognathuis and Pagrus major.
Reliability	(4) not assignable
Reference	Umezu. T. Saponins and surfactants increase water flux in fish gills. Bull Jpn Sac Sci Fish/Nippon Suisan Gakkaishi 1991;5 7(10): 1891-1896.
11.11.2004	(84)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	Carassius auratus (Fish, fresh water)
Exposure period	30 minute(s)
Unit	g/l
LC50	=1
Limit test	
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Results expressed as 1 % (vlv or w/w not known). Endpoint is behaviour (temperature selection).
Reliability	(4) not assignable
Reference	O'Connor, C.S., Crawshaw, L.I., Bedichek, R.C., Crabbe, J.C.The effect of ethanol on temperature selection in the goldfish, Carassius auratus. Pharmacal Biochem Behav 1988;29(2):243-248.
11.11.2004	(85)

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Preferred value

Test Substance:	n-Butyl Alcohol
Method:	OECD 203, USEPA TSCA 40 CFR 797.1400
Year (guideline):	1992, 1994
Type (test type):	Static Fish Acute Toxicity Test
GLP:	Yes
Year (study performed)	1998
Species:	Fathead minnow (Pimephales promelas)
Analytical Monitoring:	Yes
Exposure Period:	96 Hours
Statistical Method:	(FT - ME)* Moving Average Method
Note:	Test solutions were prepared by diluting a 50-mg/mL stock solution of n-butyl alcohol (99.9% purity) with moderately hard, filtered [0.2 mm] well water to nominal concentrations of 389, 648, 1080, 1800, and 3000 mg/L. Stock solution was. also prepared with well water. Test vessels were 19-L glass aquaria containing approximately 15 L (12-cm depth) of test solution. Two replicate test vessels were maintained for each treatment and control (dilution water) group. Vessels were covered and maintained in an environmental chamber for the test duration at 22 ±2 °C with a 16-hour light: 8-hour dark photoperiod (381 lux). Water samples for analytical verification were collected from each replicate of the control and treatments at test initiation and termination. Dissolved oxygen exceeded 60% saturation and pH ranged from 7.8 to 8.6. Temperature ranged from 22.2 to. 22.8 °C. Dilution water total organic carbon was <1 mg C/L. Total hardness, alkalinity, acidity, and specific conductance of dilution water were 132 mg/L as CaCO3, 178 mg/L as CaCO3, 20 mg/L as CaCO3, and 310 mmhos/cm, respectively. Fish were obtained from in-house cultures. Twenty minnows (10 per replicate) were exposed to each test concentration and control (dilution water). Average length of 10 control fish at test termination was 25 mm (range: 21 to 28 mm). Average weight (blotted dry) was 0.34 g (0.16 to 0.50 g). Loading was 0.23 g fish/L in test vessels.
Results:	(FT - RS) 96-hour LC50 was 1376 mg/L (95% CL: 1216 and 1587 mg/L) based on mean measured concentrations
Reliability:	(1) Valid without restrictions
Reference:	Wong, D.C.L, P.B. Dorn, and J.P. Salanitro. 1998. Aquatic

Toxicity of Four Oxy-Solvents.Equilon Enterprises, LLC Technical Information Record WTC-3520.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species Fathead Minnow (Pimepheles promelas)
Test method: Static test in Lake Superior Water or reconstituted laboratory water
Type (test type): static
Exposure Period: 96 Hr.
Results: LC50 1910 mg/l (Lake Superior water)
96 HR LCso 1940 mg/L (reconstituted laboratory water)
Reliability: (2) valid with restrictions, not all study information available
Reference: Mattson V.R., Arthur J. W. and Walbridge C. T. Acute toxicity of selected organic compounds to fathead minnows. Duluth (MN.) EPA Environ. Res. Lab., EPA-600/3-76-097, 1976.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species Fathead Minnow (Pimepheles promelas)
Test method:

Type (test type): static
GLP: No
Exposure Period: 96 Hr.
Results: LC50 1400 mg/l
Reliability: (2) valid with restrictions, not all study information available
Reference: Union Carbide Corporation, 1992b, Ecological Effects Data on Carbide Products and Process Chemicals. South Charleston, WV, 25303. (6.12.92).

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species Fathead Minnow (Pimephe/es pro me/as)
Test method:

Type (test type): static
GLP: No
Exposure Period: 96 Hr.
Results: LC50 1730 mg/l

Reliability: (2) valid with restrictions, not all study information available
Reference: Brooke, L.T., D.L. Call, D.L Geiger, and C.E. Northcott. 1984. Acute Toxicities of Organic Chemicals to Fathead Minnows

(Pimephales promelas), Vol. L Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species Bleak (Alburnus alburnus)
Test method:

Type (test type): static
GLP: No
Exposure Period:
Methods: Six concentrations (not specified) plus a control were prepared using 10 fish in each of two replicates. Concentrations were not measured and pH was not controlled. Wild caught bleaks of about 8 cm were used and fed until 48-h before testing. Testing occurred in 70-liter aquaria with 60-liter natural brackish water pumped into the laboratory from a nearby bay on the Baltic Sea. Test water had a salinity of 7 ppth, alkalinity of 1.5 meqv/L and a pH of 7.8. DO was maintained at 5 mg/L or higher and the temperature was controlled at 10"C. Lighting was 12 hr each light/dark. Mortality was recorded daily. Effect concentrations

were calculated using the graphical method described by Litchfield and Wilcoxon.
Result: 96 Hr. LCso 1730 mg/l
Reliability: (2) valid with restrictions, not all study information available
Reference: Bengtsson B. E., Renberg L., Tarkpea M. Molecular Structure and Aquatic Toxicity: an Example with C 1 -C 13 Aliphatic Alcohols. Chemosphere 13(5/6):613-622. 1984.

Linden E, Bengtsson B-E, Svanberg O., Sundstrom G. 1979. The acute toxicity of 78 chemicals and pesticide formulations against two. brackish water organisms, the Bleak (Alburnus alburnus) and the harpacticoid Nitocra spinipes. Chemosphere 11/12: 843-851.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: yes
LC50: = 97.2 - 97.5
Limit Test: no

Method: other: USEPA 1975.
Year: 1983
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Remark: Two papers (Veith et al 1983 a,b) appear to report the same study altough the LC50 values differ slightly, giving the range of LC50 values shown. The focus of these papers was to describe the relationship between experimentally obtained 96-h LC50 values for fathead minnows and the n-octanol/water partition coefficient.

Result: RESULTS: EXPOSED
LC50 = 97.2 - 97.5 mg/l
Based on measured concentrations
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
The publication indicates all concentrations were monitored daily using analytical methods, however, no results are included.

Test condition: TEST ORGANISMS
Strain: Pimephales promelas
Supplier: Environmental Research Laboratory-Duluth culture
Weight: 0.12 g
Age: 30 days old
Feeding: not reported
Pretreatment: not reported
Feeding during test: none
Control group: 2 replicates
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Lake Superior
Aeration: not reported
Alkalinity: 42.2 mg/L
Hardness: 56.3 mg/L $CaCO_3$
Conductance: Not reported
TEST SYSTEM
Concentrations: 5 different concentrations
Renewal of test solution: not reported
Exposure vessel type: Test tanks
Number of replicates: 2
Fish per replicate: 2

Test temperature: 25 C
Dissolved oxygen: > 60% of saturation
pH mean: 7.5
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported
TEST PARAMETER: Mortality
SAMPLING: Deaths recorded at 1, 3, 6, 12, 24, 48, 72 and 96h.
MONITORING OF TEST SUBSTANCE CONCENTRATION: Concentrations of chemicals in water were measured in each tank throughout the test, although analysis results were not provided.

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Veith, G.D., Call, D.J., and Brooke, L.T. 1983a. Estimating the acute toxicity of narcotic chemicals to fathead minnows. In: Bishop, W.E., Cardwell, R.D., and Heidolph, B.B. (eds.). Aquatic Toxicology and Hazard Assessment: Sixth Symposium. ASTM STP 802. American Society for Testing and Materials, Philadelphia.

Veith, G.D., Call, D.J., and Brooke, L.T. 1983b. Structure-toxicity relationships for the fathead minnow, Pimephales promelas: Narcotic industrial chemicals. Can. J. Fish. Aquat. Sci. 40:743-748.

21-DEC-2005 (75) (76)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: yes
LC50: = 117 - 126
Limit Test: no

Method: other: ASTM 1980
Year: 1985
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Remark: Flow-through toxicity tests were conducted with a geometric series (0.8 dilution factor) of toxicant concentrations for all tests. Test water was maintained at 25 degree C and pH 7.6. Successive batches of five fry or juveniles were added to

each treatment and control chamber, providing a total of 20 test organisms per treatment level.
The test was performed in 1985.

Result: RESULTS: EXPOSED
LC50 = 126 mg/l for fry
LC50 = 117 mg/l for juveniles
Based on measured concentrations
RESULTS: CONTROL
Number/% showing adverse effects: No control mortality in tests with juveniles and less than 10% in tests with fry
(refers to all 27 chemicals tested in study)

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) but showing greater toxicity are available

Reference: Broderius, S. and Kahl, M. 1985. Acute toxicity of organic chemical mixtures to the fathead minnow. Aquatic Toxicology 6:307-322.

19-JUL-2005 (16)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC0: = 30
LC50: = 55
LC100: = 100
Limit Test: no
Method: other
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Method: German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on fish-fish test (L15).
Test method corresponds to OECD Guideline 203.

Remark: Static exposures. Endpoint was mortality.
This information is from a 1 page summary of the full report but an OECD standard method was used. 10 animals per concentration.
Test was carried out prior to 1999.

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing lesser toxicity but carried out under flow-through conditions and using measured concentrations are available

Reference: Henkel KGaA. 1999t. Biological Research and Product

Safety/Ecology: unpublished results; test substance registration No. 7198. Acute fish - hexanol.
10-AUG-2005 (26)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: static
Species: Alburnus alburnus (Fish, estuary)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC50: = 120
Limit Test: no

Method: other
Year: 1984
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Remark: Fish from the Baltic Sea were placed into glass tanks containing water in groups of ten. The alcohol was then added to the tanks in a logarithmic series.
This entry was originally reported in Linden et al 1979. However, the later report (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
Result: RESULTS: EXPOSED
LC50 = 120 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: not reported
Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) but showing greater toxicity are available
Reference: Bengtsson, B., Renberg, L., and Tarkpea, M. 1984. Molecular structure and aquatic toxicity-An example with C1-C13 aliphatic alcohols. Chemosphere 13(5/6):613-622.

Linden, E., Bengtsson, B.E., Svanberg, O., and Sundstrom, G. 1979. The acute toxicity of 78 chemicals and pesticide formulations against two brackish water organisms. The bleak (Alburnus alburnus) and the harpaticoid Nitocra spinipes. Chemosphere 11-12:843-851.
19-JUL-2005 (9) (34)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: = 144

Method: other: not specified
Year: 1982
GLP: no data
Test Substance: >95% 1-hexanol (111-27-3)
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
Reference: Wellens, H. 1982. Comparison of the Sensitivity of Brachydanio rerio and Leuciscus idus by Testing the Fish Tosicity of Chemicals and Wastewaters. Z. Wasser Abwasser Forsch. Vol.15, No. 2, Pgs. 49-52.
20-OCT-2005 (80)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Unit: mg/l
Analytical monitoring: no
LC50: = 63.4 calculated

Method: other
Year: 2005
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted. input to this model is the compositional breakdown.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (2)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: yes
LC50: = 13.3 - 13.5
Limit Test: no

Method: other: ASTM 1980.
Year: 1983
GLP: yes
Test substance: > 90% 1-octanol (111-87-5)

Remark: Both Veith et al. (1983a and 1983b) citations have the same authors and report the same data. In addition, the results appear to be repeated in the studies by Brooke et al. 1984 and Broderius and Kahl 1985. Veith reports results for juveniles, Brooke reports results for fry and Broderius reports results for both. Broderius has been chosen as the representative study as this provides the most detail with regard to test results. The publications indicate that test concentrations were monitored daily using analytical methods, however the results are not provided.
Result: RESULTS: EXPOSED
LC50 = 13.3 (12.6 - 14.4) mg/l for fry
LC50 = 13.5 (12.2 - 15.0) mg/l for juveniles
Based on measured concentrations
RESULTS: CONTROL
Number/% showing adverse effects: No control mortality in tests with juveniles and less than 10% in tests with fry (refers to all 27 chemicals tested in study)
Test condition: TEST ORGANISMS
Strain: Fathead minnow
Supplier: Not reported
Age: Newly hatched fry were < 24 hours old and juvenile fathead minnows 28 to 34 days old
Weight: 0.12 g (juveniles)
Feeding: Spawning stock and juveniles were cultured on recently hatched brine shrimp nauplii (Artemia sp.) and

frozen adult brine shrimp
Pretreatment: Acclimated to test chambers for 2-3 hours prior to introduction of toxicants
Feeding during test: none
Control group: 1 control group (5 fish)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: not reported
Concentration of vehicle/solvent: not reported
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Lake Superior
Aeration: Aeration in head water reservoirs
Alkalinity: 44.0 mg/l as $CaCO_3$
Hardness: 44.6 mg/l
Conductance: not reported
TEST SYSTEM
Concentrations: not reported
Renewal of test solution: water replacement 2-4 h (25 ml/min)
Exposure vessel type: Glass chambers with silicone sealant
Number of replicates: 1
Fish per replicate: 5
Test temperature: 25 C
Dissolved oxygen: > 80% saturation
pH mean: 7.6
Adjustment of pH: not reported
Intensity of irradiation: 22 to 38 lumens/sq ft
Photoperiod: Illuminated with wide spectrum fluorescent bulbs for 16 h daily
TEST PARAMETER: lethality
SAMPLING: mortalities recorded daily
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported but publication indicates daily analytical monitoring was conducted

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Broderius, S. and Kahl, M. 1985. Acute toxicity of organic chemical mixtures to the fathead minnow. Aquatic Toxicology 6:307-322.

Brooke, L.T., Call, D.J., Geiger, D.L., and Northeadhcott, C.E. 1984. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas). Center for Lake Superior Environmental Studies, University of Wisconsin-Superior.

Veith, G.D., Call, D.J., and Brooke, L.T. 1983a.
Estimating the acute toxicity of narcotic chemicals to fathead minnows. In: Bishop, W.E., Cardwell, R.D., and Heidolph, B.B. (eds.). Aquatic Toxicology and Hazard Assessment: Sixth Symposium. ASTM STP 802. American Society for Testing and Materials, Philadelphia.

Veith, G.D., Call, D.J., and Brooke, L.T. 1983b.
Structure-toxicity relationships for the fathead minnow, Pimephales promelas: Narcotic industrial chemicals. Can. J. Fish. Aquat. Sci. 40:743-748.
19-JUL-2005 (29) (30) (120) (121)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: semistatic
Species: Alburnus alburnus (Fish, estuary)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no data
LC50: = 16
Limit Test: no

Method: other
Year: 1984
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Method: The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Ten fish were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
Remark: This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
The earlier study reports the LC50 = 15-17 mg/l
Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) but with greater toxicity are available
Reference: Bengtsson, B., Renberg, L., and Tarkpea, M. 1984.
Molecular structure and aquatic toxicity-An example with C1-C13 aliphatic alcohols. Chemosphere 13(5/6):613-622.

Linden, E., Bengtsson, B.E., Svanberg, O., and Sundstrom, G.

1979. The acute toxicity of 78 chemicals and pesticide formulations against two brackish water organisms. The bleak (Alburnus alburnus) and the harpaticoid Nitocra spinipes. Chemosphere 11-12:843-851.

19-JUL-2005 (19) (77)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l
Analytical monitoring: no data
LC0: = 10
LC50: = 17
LC100: = 30
Limit Test: no

Method: other
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Method: German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on fish-fish test (L15). Test method corresponds to OECD Guideline 203.
Remark: This information is from a 1 page summary of the full report but an OECD standard method was used. 10 fish per concentration. The test method used corresponds to OECD Guideline 203. Mortalities were recorded at 24 hour intervals.
Reliability: (2) valid with restrictions
Reference: Henkel KGaA. 1999h. Biological Research and Product Safety/Ecology: unpublished results; test substance registration No. 7199. Acute fish toxicity with 1-octanol.

20-OCT-2005 (52)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no
NOEC: = 3.2
LC50: = 18

Limit Test: no

Method: other
Year: 1996
GLP: no
Test substance: > 90% 1-octanol (111-87-5)

Method: In this preliminary toxic screen, groups of five fish were exposed to the test substance at nominal concentrations of 0.1, 0.32, 1, 3.2, 10, 32, and 100 mg/L. Control groups of fish were placed into dilution water alone or dilution water containing HCO-40 at the same level as in the test medium at the highest concentration. Observations of the fish were made on at least 24-hour intervals.
Result: Sublethal, treatment-related effects were noted at 10 mg/L and higher concentrations and included hyperventilation, darkened pigmentation, lethargy and loss of coordination. All affected fish showed symptoms within 15 minutes of exposure.
Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
Reference: Huntingdon Life Sciences Ltd. 1996g. Kalcohl 0898: Acute toxicity to rainbow trout (preliminary toxicity screen). Final report. Report No. 96/KAS218/0415.
19-JUL-2005 (60)

<u>1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)</u>

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:**
LC0: = 8
LC50: = 16
LC100: = 33
Test Substance: > 90% 1-octanol (111-87-5)
Method: other: Bestimmung der Wirkung von Wasserinhaltsstoffen auf

Remark: Toxicity tested in two different laboratories under comparable conditions; data of Luedemann.
Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the

CAS number.
Reference: Juhnke, I. & Luedemann, D., Z. Wasser Abwasser Forsch. 11, 161-164 (1978).
17-OCT-2005 (69)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:**
LC50: = 17.7

Method: other: No particulars of test method given.
Test substance: > 90% 1-octanol (111-87-5)

Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
Reference: McKim, J.M. et al., Environ. Toxicol. Chem. 6, 295-312 (1987).
17-OCT-2005 (80)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:**
LC0: 16
LC50: 20
LC100: 23

Method: other: Bestimmung der Wirkung von Wasserinhaltsstoffen auf
Test substance: > 90% 1-octanol (111-87-5)

Remark: Toxicity tested in two different laboratories under comparable conditions; data of Juhnke.
Source: Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
Reference: Juhnke, I. & Luedemann, D., Z. Wasser Abwasser Forsch. 11, 161-164 (1978).

20-OCT-2005 (69)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Unit: mg/l **Analytical monitoring:** no
LC50: = 15 calculated

Method: other
Year: 2005
GLP: no
Test substance: > 90% 1-octanol (111-87-5)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (4)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: = 2.3
Limit Test: no

Method: other: USEPA 1975.
Year: 1983
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Remark: Both Veith et al. citations (1983a and 1983b) have the same

authors and report the same data. It is likely this is the same study as reported in Brooke et al 1994. Veith reports results for juveniles and Brooke reports results for fry. The publication indicates that test concentrations were monitored daily, however, the results are not provided.

Result: RESULTS: EXPOSED
LC50 = 2.3 mg/l
Based on measured concentrations
RESULTS: CONTROL
Number/% showing adverse effects: not reported
The publication indicates all concentrations were monitored daily using analytical methods, however, no results are included.

Test condition: TEST ORGANISMS
Strain: Pimephales promelas
Supplier: Environmental Research Laboratory-Duluth culture
Weight: 0.12 g
Age: 30 days old
Feeding: not reported
Pretreatment: not reported
Feeding during test: none
Control group: 2 replicates
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Lake Superior
Aeration: not reported
Alkalinity: 42.2 mg/L
Hardness: 56.3 mg/L $CaCO_3$
Conductance: Not reported
TEST SYSTEM
Concentrations: 5 different concentrations
Renewal of test solution: not reported
Exposure vessel type: Test tanks
Number of replicates: 2
Fish per replicate: 2
Test temperature: 25 C
Dissolved oxygen: > 60% of saturation
pH mean: 7.5
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported
TEST PARAMETER: Mortality

SAMPLING: Deaths recorded at 1, 3, 6, 12, 24, 48, 72 and 96h.
MONITORING OF TEST SUBSTANCE CONCENTRATION: Concentrations of chemicals in water were measured in each tank throughout the test, although analysis results were not provided.

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Brooke, L.T., Call, D.J., Geiger, D.L., and Northeadhcott, C.E. 1984. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas). Center for Lake Superior Environmental Studies, University of Wisconsin-Superior.

Veith, G.D., Call, D.J., and Brooke, L.T. 1983a. Estimating the acute toxicity of narcotic chemicals to fathead minnows. In: Bishop, W.E., Cardwell, R.D., and Heidolph, B.B. (eds.). Aquatic Toxicology and Hazard Assessment: Sixth Symposium. ASTM STP 802. American Society for Testing and Materials, Philadelphia.

Veith, G.D., Call, D.J., and Brooke, L.T. 1983b. Structure-toxicity relationships for the fathead minnow, Pimephales promelas: Narcotic industrial chemicals. Can. J. Fish. Aquat. Sci. 40:743-748.

21-DEC-2005 (19) (98) (99)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: static
Species: other: Salmo gairdneri (rainbow trout) and Lepomis macrochirus (bluegill)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC50: > 4.2 - 5.6
Limit Test: no

Method: other: USEPA 1975.
Year: 1975
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Remark: Test compound was added to each jar in a solution of acetone. A control which contained the greatest amount of acetone introduced into any test was conducted. Ten fish were exposed to a range of concentrations (2.4-10 mg/L for Rainbow trout and 3.2-10 mg/l for bluegill) and a control.

Static bioassays were conducted at 21 C for the bluegill and at 12 C for the rainbow trout, both at a pH of 7.1. The bluegill had a mean weight and length of 1.0 g and 36 mm and the rainbow trout weighed 1.2 g and was 56 mm in length.

Result: The 96-h LC50 was 5.05 for bluegill and >4.2 - < 5.6 for rainbow trout. The highest concentrations at which there was no discernible effect (NOEC) during the 96-h bioassay was 3.2 mg/l for the bluegill and 2.4 mg/l for the rainbow trout. Prior to death, fish generally became dark and lethargic and lost equilibrium. No mortalities were observed in any of the control groups.

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available

Reference: E.G.& G. Bionomics. 1975. Acute toxicity of two Conoco compounds to bluegill (lepomis macrochirus) and rainbow trout (Salmo gairdneri). Bioassay report submitted to Conoco Chemicals, Ponca City, Oklahoma.

17-OCT-2005 (24)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no
NOEC: = 1
LC50: = 5.7
Limit Test: no

Method: other
Year: 1996
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Method: In this preliminary toxicity screen, groups of five fish were exposed to the test substance at nominal concentrations of 0.1, 0.32, 1, 3.2, 10, 32, and 100 mg/L. Control groups of fish were placed into dilution water alone or dilution water containing HCO-40 at the same level as in the test medium at the highest concentration. Observations of the fish were made at 24-hour intervals.

Result: Sublethal, treatment-related effects were noted at 3.2 mg/L and higher concentrations and included hyperventilation, darkened pigmentation, lethargy and loss of coordination.

All fish were adversely affected within 15 minutes of exposure.

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available

Reference: Huntingdon Life Sciences Ltd. 1996h. Kalcohl 1095: Acute toxicity to rainbow trout (preliminary toxicity screen). Final report. Report No. 96/KAS224/0416.

19-JUL-2005 (49)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: static
Species: Alburnus alburnus (Fish, estuary)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC50: = 7.2
Limit Test: no

Method: other
Year: 1979
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Method: The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Ten fish were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.

Remark: This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) but with greater toxicity are available

Reference: Bengtsson, B., Renberg, L., and Tarkpea, M. 1984. Molecular structure and aquatic toxicity-An example with C1-C13 aliphatic alcohols. Chemosphere 13(5/6):613-622.

Linden, E., Bengtsson, B.E., Svanberg, O., and Sundstrom, G. 1979. The acute toxicity of 78 chemicals and pesticide formulations against two brackish water organisms. The bleak (Alburnus alburnus) and the harpaticoid Nitocra spinipes. Chemosphere 11-12:843-851.

19-JUL-2005 (15) (62)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l
Analytical monitoring: no data
LC0: = 5.6
LC50: = 8.4
LC100: = 11
Limit Test: no

Method: other
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Method: German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on fish-fish test (L15). Test method corresponds to OECD Guideline 203.
Remark: This information is from a 1 page summary of the full report but an OECD standard method was used. 10 fish per concentration. Mortalities are recorded at least at 24 hour intervals.
Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
Reference: Henkel KGaA. 1999n. Biological Research and Product Safety/Ecology: unpublished results; test substance registration No. 6368. Fish acute with 1-decanol. August 1999.
19-JUL-2005 (44)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:**
LC0: = .4 - 1
LC50: = .6 - 3.2
LC100: = .8 - 10

Test substance: > 90% 1-decanol (112-30-1)

Reliability: (4) not assignable
Not key study: Other studies with higher reliability score are available.

Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.
19-JUL-2005 (100)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Unit: mg/l **Analytical monitoring:** no
LC50: = 1.9 calculated

Method: other
Year: 2005
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (3)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: = 1.01
Limit Test: no

Method: other: USEPA 1975
Year: 1983
GLP: no data
Test substance: other TS: Dodecanol (112-53-8)

Result: RESULTS: EXPOSED
LC50 = 1.01 mg/l
Based on measured results
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
The publication indicates all concentrations were monitored daily using analytical methods, however, no results are included.

Source: Veith et al. 1983a; Veith et al. 1983b.

Test condition: TEST ORGANISMS
Strain: Pimephales promelas
Supplier: Environmental Research Laboratory-Duluth culture
Weight: 0.12 g
Age: 30 days old
Feeding: not reported
Pretreatment: not reported
Feeding during test: none
Control group: 2 replicates
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Lake Superior
Aeration: not reported
Alkalinity: 42.2 mg/L
Hardness: 56.3 mg/L $CaCO_3$
Conductance: Not reported
TEST SYSTEM
Concentrations: 5 different concentrations
Renewal of test solution: not reported
Exposure vessel type: Test tanks
Number of replicates: 2
Fish per replicate: 2
Test temperature: 25 C
Dissolved oxygen: > 60% of saturation
pH mean: 7.5
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported

TEST PARAMETER: Mortality
SAMPLING: Deaths recorded at 1, 3, 6, 12, 24, 48, 72 and 96h.

MONITORING OF TEST SUBSTANCE CONCENTRATION: Concentrations of chemicals in water were measured in each tank throughout the test.

Reliability: (2) valid with restrictions

Flag: Critical study for SIDS endpoint

Reference: Veith, G.D., Call, D.J., and Brooke, L.T. 1983a. Estimating the acute toxicity of narcotic chemicals to fathead minnows. In: Bishop, W.E., Cardwell, R.D., and Heidolph, B.B. (eds.). Aquatic Toxicology and Hazard Assessment: Sixth Symposium. ASTM STP 802. American Society for Testing and Materials, Philadelphia.

Veith, G.D., Call, D.J., and Brooke, L.T. 1983b. Structure-toxicity relationships for the fathead minnow, Pimephales promelas: Narcotic industrial chemicals. Can. J. Fish. Aquat. Sci. 40:743-748.

12-MAR-2004 (23) (24)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)

Type: semistatic

Species: Oncorhynchus mykiss (Fish, fresh water)

Exposure period: 96 hour(s)

Unit: mg/l **Analytical monitoring:** no

NOEC: >= 1

LC50: > 1

Limit Test: yes

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"

Year: 1996

GLP: yes

Test substance: other TS: Dodecanol (112-53-8)

Method: 2 groups of 10 fish were exposed to an aqueous dispersion of the test material at a single concentration of 1.0 mg/l. Mortalities and sub-lethal effects of exposure were determined at 3 and 6 hours after the start of the test and then daily until termination at 96 hours.

Source: Wetton 1996a.

Test substance: Corresponds to tradename Kalcol 2098.

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available

Reference: Wetton, P.M. 1996a. Kalcol 2098: Acute toxicity to rainbow trout (Oncorhynchus mykiss). SPL Project Number 140/592.

12-MAR-2004 (28)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Type: semistatic
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: yes
NOEC: >= 1
LC50: > 1
Limit Test: yes

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1996
GLP: yes
Test substance: > 95% 1-Tetradecanol (112-72-1)

Remark: The concentration of 1.0 mg/L was reported to be the highest attainable test concentration due to the limited water solubility, therefore the LC50 was not achieved at the solubility limit, (although 1 mg/l is greater than the measured solubility in pure water).
Result: RESULTS: EXPOSED
NOEC > 1.0 mg/l
LC50 > 1.0 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0
Test condition: TEST ORGANISMS
Strain: Oncorhynchus mykiss
Supplier: Parkwood Trout Farm, Harrietsham, Kent UK
Weight: 0.90 g
Feeding: Commercial trout pellets
Pretreatment: Fish acclimatised to test conditions for 7 days prior to test
Feeding during test: Discontinued 23 hours prior to test
Control group: Control and solvent control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Tetrahydrofuran
Concentration of vehicle, solvent: 100 uL/L
STABILITY OF TEST CHEMICAL SOLUTIONS: Not determined
DILUTION WATER
Source: Dechlorinated laboratory tap water
Aeration: Test vessels were aerated during test
Alkalinity: 137 mg/l

Hardness: 259 mg/l CaCO3
Conductance: 627 uS/cm
TEST SYSTEM
Concentrations: 1.0 mg/l
Renewal of test solution: Daily
Exposure vessel type: 20 l glass vessels
Number of replicates: 2
Fish per replicate: 10
Test temperature: 14 C
Dissolved oxygen: = 9.0 - 9.9 mg O2/l
pH mean: 7.6-8.2
TEST PARAMETER: Mortality
SAMPLING: Monitoring of test animals for mortality and
sub-lethal effects at 3, 6, 24, 48 and 96 hours
MONITORING OF TEST SUBSTANCE CONCENTRATION: Not reported

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Wetton, P.M. 1996b. Kalcol 4098: Acute toxicity to rainbow trout (Oncorhynchus mykiss). SPL Project Number 140/599.

17-OCT-2005 (82)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Type: semistatic
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC0: = 10000
LC50: > 10000
Limit Test: no

Method: Directive 92/69/EEC, C.1
Year: 1994
GLP: yes
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: RESULTS: EXPOSED
LC50 = >10000 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: none

Nature of adverse effects: mortality or sublethal effects
No mortality or sublethal effects were seen
Substance loading is well above the water solubility limit.

Test condition: TEST ORGANISMS
Strain: Brachydanio rerio
Supplier: Westaquarium
Wild caught: no
Age/size/weight/loading: not reported
Feeding: Altromin N 1324
Pretreatment: none
Feeding during test: none
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: none
Vehicle, solvent: none
Other procedures: test substance was directly weighed into test vessels followed by 10 sec treatment with blender to disperse poorly soluble test substance.
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
REFERENCE SUBSTANCE: none
TEST SYSTEM
Concentrations: 0, 1000, 3000, 10000 mg/l
Renewal of test solution: daily
Exposure vessel type: 5 L aquarium
Number of replicates: 1
Fish per replicate: 10
Test temperature: 20.5 - 22.5C
Dissolved oxygen: 63-95% saturation
pH mean: 7.9-9.4
Adjustment of pH: not reported
Photoperiod: not reported
DURATION OF THE TEST: 96 h
TEST PARAMETER: mortality

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) but tested closer to the limit of water solubility are available

Reference: Stelter 1994. 1-tetradecanol: Acute toxicity: Fish. Biological research and Product Safety/Ecology: Unpublished results; test substance registration no. 930812; Henkel KGaA; Report No. R9400455; (with English summary report no. R9901350).

11-JAN-2005 (70)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Unit: mg/l **Analytical monitoring:** no
LC50: > 100 calculated

Method: other

Year: 2005
GLP: no
Test substance: > 95% 1-Tetradecanol (112-72-1)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
Result: Predicted to be non-toxic at the limit of solubility
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (4)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Type: semistatic
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no data
NOEC: >= .4
LC50: > .4
Limit Test: yes

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1996
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: The solubility of C16 alcohol (hexadecanol) is about 0.01 mg/l, therefore the LC50 was not achieved at the solubility limit.
Result: RESULTS: EXPOSED
Based on nominal concentrations
RESULTS: CONTROL

Number/% showing adverse effects: 0

Source: Wetton 1996c.

Test condition: TEST ORGANISMS
Strain: Oncorhynchus mykiss
Supplier: Donnington Fish Farm, Upper Swell, Gloucestershire, UK
Weight: 1.20 g
Feeding: Commercial trout pellets
Pretreatment: Acclimatised to test conditions for 1 week prior to test
Feeding during test: None
Control group: 1 control and 1 solvent control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Tetrahydrofuran
Concentration of vehicle, solvent: 100 uL/L
STABILITY OF TEST CHEMICAL SOLUTION
not reported
DILUTION WATER
Source: Dechlorinated laboratory tap water
Aeration: Test vessels aerated via narrow bore glass tubes
Alkalinity: 80 mg/l
Hardness: 136 mg/l CaCO3
Conductance: 405 uS/cm
TEST SYSTEM
Concentrations: 0.4 mg/l
Renewal of test solution: Daily
Exposure vessel type: 20 l glass vessels
Number of replicates: 2
Fish per replicate: 10
Test temperature: 13-14 C
Dissolved oxygen: 9.2 - 10.1 mg O2/l
pH mean: 7.4 - 7.9
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: 16 hours light and 8 hours darkness
TEST PARAMETER: Mortality
SAMPLING: Mortalities and adverse reactions to exposure were recorded at 3, 6, 24, 48, 72 and 96 hours
MONITORING OF TEST SUBSTANCE CONCENTRATION: Not reported

Reliability: (2) valid with restrictions

Flag: Critical study for SIDS endpoint

Reference: Wetton, P.M. 1996c. Kalcol 6098: Acute toxicity to rainbow trout (Oncorhynchus mykiss). SPL Project Number 140/500.

17-OCT-2005 (100)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: semistatic
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: yes
LC50: > 10
Limit Test: no

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1995
GLP: no data
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: Five acute toxicity tests were conducted with hexadecanol using four different preparation methods. None of the tests resulted in significant mortality due to the action of hexadecanol. Although the deaths in the control (typicaly 10-30%) complicate the interpretation, the data demonstrate that the 96 hour LC50 was greater than the highest concentration tested (10 mg/L). This is about 1000 times the water solubility of hexadecanol.
Source: Unilever, 1995.
Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) but tested closer to the limit of water solubility available
Reference: Unilever. 1995. Bioavailability: Research Contract Sponsored by the Department of the Environment. Final Report. June 1995.
21-JUL-2005 (90)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: static
Species: Oncorhynchus kisutch (Fish, fresh water, marine)
Unit: mg/l
Analytical monitoring:
LC0: > 10
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: keine toxische Wirkung bei 10 mg/l
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: T = 11 Grad C; pH 7.2
Reliability: (4) not assignable

This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.

Reference: MacPhee, C. & Ruelle, R., "Lethal effects of 1888 chemicals upon four species of fish from western North America". Idaho For. Wildl. Range Exp. Stn. Bull. 3, 1-112 (1969).

17-OCT-2005 (57)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: static
Species: Oncorhynchus tschawytscha (Fish, fresh water, marine)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:**
LC0: > 10
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: keine toxische Wirkung bei einer Konzentration von 10 mg/l
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test condition: T = 11 Grad C; pH 7.2
Reliability: (4) not assignable

This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.

Reference: MacPhee, C. & Ruelle, R., "Lethal effects of 1888 chemicals upon four species of fish from western North America". Idaho For. Wildl. Range Exp. Stn. Bull. 3, 1-112 (1969).

17-OCT-2005 (57)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 5
Unit: mg/l **Analytical monitoring:**
LC0: = 500

Method: other: keine naeheren Angaben
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: der Stoff wurde von den Fischen aufgenommen und offenbar unveraendert ausgeschieden, die durch Filmbildung reduzierte Sauerstoffzufuhr verursachte bei den Tieren Stresserscheinungen keine toxische Wirkung bis 500 mg/l.

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test substance: Emulsion von 1-Hexadecanol in Wasser
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
Reference: Berger, B.B., J. Am. Water Works Assoc. 50, 855-858 (1958).
17-OCT-2005 (11)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: static
Species: Ptychocheilus oregonensis (Fish, fresh water)
Exposure period: 24 hour(s)
Unit: mg/l
Analytical monitoring:
LC0: > 10

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: keine toxische Wirkung bei einer Konzentration von 10 mg/l
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
Reference: MacPhee, C. & Ruelle, R., "Lethal effects of 1888 chemicals upon four species of fish from western North America". Idaho For. Wildl. Range Exp. Stn. Bull. 3, 1-112 (1969).
20-OCT-2005 (57)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: static
Species: Salmo irideus (Fish, fresh water)

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Hexadecanol has no significant effect on either respiration or total resting metabolism of Salmo irideus. When the fish were confined, oxygen consumption was increased only during the recuperation period in pure water and 2 hr following exposure to 10, 100, and 1000 ppm hexadecanol. Under semiconfinment conditions, 2-3 ppm hexadecanol had no effect on total resting metabolism.
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
Reference: Gorin, J.; Correia-Dereumaux, B.; Erb, Francoise; Harichaux, Pierre: "Study on the toxicity of higher fatty alcohols on rainbow trout (Salmo irideus). Particular study on the effects of hexacdecanol and octadecanol on the respiratory function", Bull. Fr. Piscic., 277, 163-84.
17-OCT-2005 (35)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Unit: mg/l
Analytical monitoring: no
LC50: > 100 calculated

Method: other
Year: 2005
GLP: no
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (4)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Type: semistatic
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: >= .4
LC50: > .4
Limit Test: yes

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1996
GLP: yes
Test substance: other TS: Octadecanol (112-92-5)

Remark: The solubility of octadecanol is estimated at about 0.001 mg/L, therefore the LC50 was not achieved at the solubility limit.
Result: RESULTS: EXPOSED
LC50 >0.40
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0
Source: Wetton 1996d.
Test condition: TEST ORGANISMS
Strain: Oncorhynchus mykiss
Supplier: Donnington Fish Farm, Upper Swell, Gloucestershire, UK
Weight: 1.20 g
Feeding: commercial trout pellets
Pretreatment: Fish acclimatised to test conditions for 1 week prior to test
Feeding during test: None
Control group: 1 control group and 1 solvent control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Tetrahydrofuran
Concentration of vehicle, solvent: 100 uL/L
STABILITY OF TEST CHEMICAL SOLUTIONS
Not reported
DILUTION WATER
Source: Dechlorinated laboratory tap water
Aeration: Test vessels aerated via narrow bore glass tubes
Alkalinity: 80 mg/l
Hardness: 136 mg/l CaCO3
Conductance: 382 MICSM
TEST SYSTEM
Concentrations: 0.4 mg/l
Renewal of test solution: Daily

Exposure vessel type: 20 l glass vessels
Number of replicates: 2
Fish per replicate: 10
Test temperature: 13-14 C
Dissolved oxygen: 9.2 - 10.1 mgO2/l
pH mean: 7.5 - 7.9
TEST PARAMETER: Mortality

SAMPLING: Mortalities and adverse reactions were recorded at 3, 6, 24, 48, 72 and 96 hours
MONITORING OF TEST SUBSTANCE CONCENTRATION: Not reported

Test substance: Corresponds to CAS# 112-92-5. Tradename is Kalcol 8098.
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Wetton, P.M. 1996d. Kalcol 8098: Acute toxicity to rainbow trout (Oncorhynchus mykiss). SPL Project Number 140/506.
12-MAR-2004 (16)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Type: semistatic
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no
LC0: = 10000
LC50: > 10000
Limit Test: no

Method: other: ISO 7346/II
Year: 1993
GLP: yes
Test substance: other TS: Octadecanol (112-92-5)

Result: RESULTS: EXPOSED
LC50 = >10000 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: none

Nature of adverse effects: mortality or sublethal effects
No mortality or sublethal effects were seen
Exposures were well in excess of water solubility limit.
Source: Stelter 1993.

Test condition: TEST ORGANISMS
Strain: Brachydanio rerio
Supplier: Westaquarium
Wild caught: no
Age/size/weight/loading: not reported
Feeding: Altromin N 1324
Pretreatment: none
Feeding during test: none
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: none
Vehicle, solvent: none
Other procedures: test substance was directly weighed into test vessels followed by 10 sec treatment with blender to disperse poorly soluble test substance.
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
REFERENCE SUBSTANCE: none
TEST SYSTEM
Concentrations: 0, 1000, 3000, 10000 mg/l
Renewal of test solution: daily
Exposure vessel type: 5 L aquarium
Number of replicates: 1
Fish per replicate: 10
Test temperature: 21.4 - 23.8C
Dissolved oxygen: 65-100% saturation
pH mean: 6.6-7.5
Adjustment of pH: not reported
Photoperiod: not reported
DURATION OF THE TEST: 96 h
TEST PARAMETER: mortality

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) but tested closer to the limit of water solubility are available

Reference: Stelter Dr. 1993. 1-Octadecanol: Acute toxicity: Fish. Biological research and Product Safety/Ecology: Unpublished results; test substance registration No. 920386; Henkel KGaA; Report No. R9300206; (with english summary report no. R9901351).

12-MAR-2004 (13)

<u>1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)</u>

Unit: mg/l
Analytical monitoring: no
LC50: > 100 calculated

Method: other
Year: 2005
GLP: no
Test substance: >= 90% 1-eicosanol (629-96-9)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (2)

<u>1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)</u>

Type: semistatic
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no
LL50 : > 1000
Limit Test: yes

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)

Remark: Test material was prepared as a filtered Water Accommodated Fraction (WAF) by loading test medium with the respective amount of the test item. After stirring for 23 hours, the contents were left to settle for 1h. The mixture was then filtered through 0.2 um filters to give the 1000 mg/l

loading rate filtered WAF.

Result: RESULTS: EXPOSED
LL50 > 1000 mg/l
Based on nominal loading rates
RESULTS: CONTROL
Number/% showing adverse effects: 0

Test condition: TEST ORGANISMS
Strain: Oncorhynchus mykiss
Supplier: Brow Well Fisheries, Hebden, Nr. Skipton, Yorkshire, UK
Weight: 0.89 g (mean)
Feeding: Commercial trout pellets
Pretreatment: Fish acclimatised to test conditions for 2 weeks prior to test
Feeding during test: None
Control group: 1 control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accommodated fractions
Vehicle, solvent: None
Concentration of vehicle/solvent: none
STABILITY OF TEST CHEMICAL SOLUTIONS
Not reported
DILUTION WATER
Source: Dechlorinated laboratory tap water
Aeration: Aerated vai narrow bore glass tubes
Alkalinity: Not reported
Hardness: approximately 100 mg/l CaCO3
Conductance: Not reported
TEST SYSTEM
Concentrations: 1000 mg/l
Renewal of test solution: Daily
Exposure vessel type: 20 l glass vessels
Number of replicates: 2
Fish per replicate: 7
Test temperature: 14 C
Dissolved oxygen: 9.4 - 9.9 mgO2/l
pH mean: 7.9 - 8.1
TEST PARAMETER: Mortality
SAMPLING: Mortalities and adverse reactions were recorded at 3, 6, 24, 48, 72 and 96 hours
MONITORING OF TEST SUBSTANCE CONCENTRATION: Not reported

Reliability: (2) valid with restrictions

Flag: Critical study for SIDS endpoint

Reference: Wetton, P.M. 2000. Kalcol 220-80: Acute toxicity to rainbow trout (Oncorhynchus mykiss). SPL Project Number

140/1001.
11-SEP-2005 (31)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Unit: mg/l
Analytical monitoring: no
LC50: > 100 calculated

Method: other
Year: 2005
GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (2)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Unit: mg/l **Analytical monitoring:** no
LC50: = 1.9×10^{-6} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-tetracosanol

Method: ECOSAR v0.99, USEPA (2006).

Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, 2006.
05-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Unit: mg/l **Analytical monitoring:** no
LC50: = 2.41×10^{-7} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-hexacosanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, 2006.
05-APR-2007

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Unit: mg/l **Analytical monitoring:** no
LC50: = 3.1×10^{-8} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-octacosanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, 2006.
05-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Unit: mg/l
Analytical monitoring: no
LC50: = 3.97×10^{-9} calculated

Method: other
Year: 2006
GLP: no

Test substance: 1-triacontanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, 2006.
05-APR-2007

4.2 Acute Toxicity to Aquatic Invertebrates

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Static
Species	Ceriodaphnia sp. (Crustacea)
Exposure period	48 hour(s)
Unit	mg/l
LC50	= 5012 measured/nominal
Analytical monitoring	no data
Method	other: ASTM (see ME)
Year	1987
GLP	no data
Test substance	other TS: Absolute ethanol

Remark

Method was that recommended by the American Society of Testing and Materials (19S0) Standard practice for conducting acute toxicity tests with fishes, macroinvertebrates and amphibians. ASTM Standard E729-80.
Philadelphia, Pennsylvania.

Test organism: Cerodaphnia dubia: Source not specified. Organisms were mass cultured an acclimated to temperature for at least 10 weeks and maintained in filtered, autoclaved Lake Huron water. Neonates hatched by isolated gravid females gathered by sieving.
Age: Neonates.
Control group: Dilution water controls.
Test conditions: Ethanol not discussed.
Test temperature: 24 deg C.
Exposure vessel: Covered vials, not aerated, triplicates for each concentration.
Dilution water source: See above.
Dilution water chemistry: Hardness 90 mg/I as CaCO3, Alkalinity 70 mg CaCO3, pH S,S, TOC 5580 mug/I; TDS 140,000 mug/I; Ca/Mg 2.S. Na/K 4.3.
Lighting: 646 lux +/- 85; 16 hr light, S hr dark.
Water chemistry on test: Dissolved Oxygen 8.4-10.3 mg/I, pH

	8.2-8.4. Endpoint assessment Assessed microscopically. Test design: Ten individuals per beaker, 3 replicates per concentration. Concentrations of ethanol not specified. Method of calculating mean measured concentration: Not discussed; Geometric mean LC50's calculated. Statistical method: Thompson moving averages. Species: Ceriodaphnia dubia Biological observations: Number immobilized as compared to number exposed; Not discussed. Concentration response with 95% confidence limits (LC50) 5012 mg/l (4233-6913 mg/l). Cumulative immobilization: Not discussed. Satisfactory control response?: Unknown. Cumulative immobilization: Not discussed. Satisfactory control response?: Unknown.
Result	LC50 values ranged from 6325 to 6772 mg/l at 20 degree C and from 3715 to 6076 mg/l at 24 degree C.
Test substance	Test substance was pure (absolute) ethanol (dehydrated U.S.P.).
Reliability	(2) valid with restrictions These data are regarded as reliable. Fugacity data suggests low losses would be expected by evaporation, however as no measurements made, only rated reliable with restrictions.
Flag	Critical study for SIDS endpoint
Reference	Takahashi, I.T.,Cowgill, U.M., Murphy, P.G. (1987) Comparison ot ethanol toxicity to Daphnia magna and Ceriodaphnia dubia tested at two differenttemperatures: Static acute toxicity test results. Bull. Environ. Contam. ToxicoL 39:229-236.
11.11.2004	(86)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	Daphnia magna (Crustacea)
Exposure period	48 hour(s)
Unit	mg/l
LC50	= 12340 measured/nominal
Analytical monitoring	no data

Method	other: ASTM (see ME)
Year	1987
GLP	no data
Test substance	other TS: Absolute ethanol
Remark	Biological observations: Number immobilized as compared to number exposed; Not discussed. Concentration response with 95% confidence limits (LC50) 1,2340 mg/l (11.065-13,948 mg/l). Cumulative immobilization: Not discussed. Satisfactory control response?: Unknown. Cumulative immobilization: Not discussed. Satisfactory control response?: Unknown. LC50 values ranged from 11853 to 13248 mg/l at 20 degree C and from 9268 to 14221 mg/l at 24 degree C. Method was that recommended by the American Society of Testing and Materials (1980) Standard practice for conducting acute toxicity tests with fishes, macro invertebrates and amphibians. ASTM Standard E729-80. Philadelphia, Pennsylvania. Test organism: Daphnia magna: Source not specified. Stocks maintained in adjusted, autoclaved, aerated lake Huron water for 3 years before start of study. Neonates hatched by isolated gravid females gathered by sieving. Age: Neonates. Control group: Dilution water controls. Test conditions: Ethanol not discussed. Test temperature: 20 deg C. Exposure vessel: Covered beakers, not aerated, triplicates for each concentration. Dilution water source: See above. Dilution water chemistry: Hardness 160 mg/I as CaC03, pH 8.0, TOC 5520 mug/I; TDS 289,550 mug/I; Ca/Mg 5.7. NalK 4.5. lighting: 1916 lux +/- 75; 16 hr light, 8 hr dark. Water chemistry on test: Dissolved Oxygen 7.6-8.9 mg/l, pH 7.8-8.4. Endpoint assessment: Assessed microscopically. Test design: Ten individuals per beaker, 3 replicates per concentration. Concentrations of ethanol not specified. Method of calculating mean measured concentration: Not discussed; Geometric mean lC50's calculated.

	Statistical method: Thompson moving averages.
Test substance	Test substance was pure (absolute) ethanol (dehydrated U.S.P.).
Reliability	(2) valid with restrictions These data are regarded as reliable. Fugacity data suggests low losses would be expected by evaporation, however as no measurements made, only rated reliable with restrictions.
Reference	Takahashi, I.T., Cowgill, U.M., Murphy, P.G. (1987) Comparison ot ethanol toxicity to Daphnia magna and Ceriodaphnia dubia tested at two different temperatures: Static acute toxicity test results. Bull. Environ. Contam. Toxicol. 39: 229-236.
11.11.2004	(87)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	other: not specified
Species	Artemia salina (Crustacea)
Exposure period	1 day(s)
Unit	mg/l
LC50	= 1833 measured/nominal
Analytical monitoring	no data
Method	other
Year	1994
GLP	no data
Test substance	ethanol (64-17-5)
Method	Artemia salina 24 h nauplius larvae were exposed to unspecified nominal concentrations of ethanol for 24 h.
Remark	Biological observations: Number immobilized as compared to number exposed; Not discussed. Concentration response with 95% confidence limits (LC50) 1 ,834 mg/I (1,324-2,538 mg/I). Cumulative immobilization: Not discussed. Satisfactory control response: Unknown. Cumulative immobilization: Not discussed. Satisfactory control response?: Unknown. Test organism: Artemia salina hatched from dry eggs supplied by San Francisco Bay Brand hatter hydration in distilled water. Cysts were incubated. in synthetic sea water for 24 h at 25 deg C with continuous side illumination and slight aeration. Age: 24-h-old nauplius larvae.

	Control group: Used but not described. Test conditions: Synthetic seawater was pore pared using 35% Synthetica sea salt and distilled deionized seawater. Test temperature: 25 deg C. Exposure vessel: Plastic 16 mm petri dishes. Dilution water source: See above. Dilution water chemistry: Not described. Lighting: Incubated in the dark. Water chemistry on test: Not discussed. Endpoint assessment:· Organisms considered dead if they did not move during 10 see observation. Test design: Ten larvae per dish, 3-5 replicates per concentration; experiment repeated 5 times. Concentrations of ethanol not specified. Method of calculating mean measured concentration: Nominal concentrations only. Statistical method: Litchfield and Wilcoxon.
Result	Further studies involved older larvae: 48 h LC50 850 mg/l 72 h LC50 695 mg/l Sensitivity to ethanol was therefore age-related.
Reliability	(2) valid with restrictions
Reference	Barahona-Gomariz, M.V., Sanz-Narrera, F., Sanchez-Fortun, S. Acute toxicity of organic solvents on Artemia salina. Bull Environ Contam Toxicol 1994;52(5):766-771.
11.11.2004	(88)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	Ceriodaphnia sp. (Crustacea)
Exposure period	48 hour(s)
Unit	mg/l
LC50	= 5012 measured/nominal
Analytical monitoring	no data
Method	other: ASTM (see ME)
Year	1987
GLP	no data
Test substance	other TS: Absolute ethanol
Remark	Method was that recommended by the American Society of Testing and Materials (19S0) Standard practice for conducting acute toxicity tests with fishes, macroinvertebrates and amphibians. ASTM Standard E729-80.

Philadelphia, Pennsylvania.

Test organism: Cerodaphnia dubia: Source not specified. Organisms were mass cultured an acclimated to temperature for at least 10 weeks and maintained in filtered, autoclaved Lake Huron water. Neonates hatched by isolated gravid females gathered by sieving.
Age: Neonates.
Control group: Dilution water controls.
Test conditions: Ethanol not discussed.
Test temperature: 24 deg C.
Exposure vessel: Covered vials, not aerated, triplicates for each concentration.
Dilution water source: See above.
Dilution water chemistry: Hardness 90 mg/I as CaCO3, Alkalinity 70 mg CaCO3, pH S,S, TOC 5580 mug/I; TDS 140,000 mug/I; Ca/Mg 2.S. Na/K 4.3.
Lighting: 646 lux +/- 85; 16 hr light, S hr dark.
Water chemistry on test: Dissolved Oxygen 8.4-10.3 mg/I, pH

8.2-8.4.
Endpoint assessment Assessed microscopically.
Test design: Ten individuals per beaker, 3 replicates per concentration. Concentrations of ethanol not specified.
Method of calculating mean measured concentration: Not discussed; Geometric mean LC50's calculated.

Statistical method: Thompson moving averages.
Species: Ceriodaphnia dubia

Biological observations:

Number immobilized as compared to number exposed; Not discussed.

Concentration response with 95% confidence limits (LC50) 5012 mg/l (4233-6913 mg/l).
Cumulative immobilization: Not discussed.
Satisfactory control response?: Unknown. Cumulative immobilization: Not discussed. Satisfactory control response?: Unknown.

Result LC50 values ranged from 6325 to 6772 mg/l at 20 degree C and from 3715 to 6076 mg/l at 24 degree C.

Test substance Test substance was pure (absolute) ethanol (dehydrated U.S.P.).

Reliability (2) valid with restrictions These data are regarded as reliable.

	Fugacity data suggests low losses would be expected by evaporation, however as no measurements made, only rated reliable with restrictions. Critical study for SIDS endpoint
Reference	Takahashi, I.T.,Cowgill, U.M., Murphy, P.G. (1987) Comparison of ethanol toxicity to Daphnia magna and Ceriodaphnia dubia tested at two different temperatures: Static acute toxicity test results. Bull. Environ. Contam. Toxicol. 39: 229-236.
11.11.2004	(86)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	other: Paramecium caudatum (ciliate Protozoon)
Exposure period	4 hour(s)
Unit	mg/l
LC50	= 5840
Limit test	No
Analytical monitoring	no data
Method	other
Year	1989
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Age of test species: 48hrs Control group: None mentioned. A number of other solvents tested as well as pesticide compounds. Test conditions: Stock solutions split-pea medium. Test temperature range 25 deg C +/- 2 deg. Exposure vessel: not specified. Test in 100 ml containing 1 ml of culture containing 1,500-2000 stationary phase organisms/ml. Dilution water source: not specified. Dilution water chemistry: Not measured. Lighting: not specified. Water chemistry on test: Not measured. Medium was Chalkley's isotonic inorganic salt (Patterson, 1982) Endpoint assessment: lethal concentration at which all animals died in 10 mins; death indicated by lack of swimming and or rupture of cell. Also, 4 hr median lethal concentration (LC50). Replicates: 5 Number of concentrations for 4hr LC50 evaluation: 0.1, 0.2, 0.4, 0.8, 1.2, 2% v/v (790 to 15,800 mg/l)
Result	10 minute LC50=5% v/v (39,OOOmg/l)
Test substance	commercial absolute alcohol
Reliability	(2) valid with restrictions Method details not comprehensive. Results available for each concentration but only in graphical

	form. However, study sufficiently well reported to rate reliable.
Reference	Rajini, P.S., Krishnakumari, M.K., Majumder, SK Cytotoxicity of certain organic solvents and organophosphorus insecticides to the ciliated Protozoan Paramecium caudatum. Microbios 1989;59:157-163.
17.11.2004	(89)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Static
Species	other aquatic crustacea: Palaemonetes kadiakensis
Exposure period	18 hour(s)
Unit	g/L
EC50	= 10.1 measured/nominal
Analytical monitoring	No
Method	
Year	1981
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Organisms exposed to 4 concentrations of ethanol in the range 1% v/v to 2% vivo Test conducted at 23 deg. C.
Remark	Biological observations: Number immobilized as compared to number exposed; mortality ranged from 0 to 100%. Concentration response with 95% confidence limits (LC50) 1.28% v/v (1.18-1.38). Cumulative immobilization: Not discussed. Satisfactory control response?: Unknown. Test organism: Palaeomonetes kadlakensis caught in a nearby lake. Age: Juveniles. Control group: None mentioned. Test conditions: Stock solutions preparation not discussed. Test temperature range 23 deg C +/- 1 deg. Exposure vessel: 2 litre beakers containing 100 ml test medium. Each dilution tested in duplicate. Dilution water source: Aerated deionized deep well water. Dilution water chemistry: Not measured. Lighting: 1 h of typical fluorescent light illumination, 15.5 h 10% normal illumination then 1.5 h typical illumination. Water chemistry on test: Not measured. Endpoint assessment: Organisms considered dead if they did not respond to light, sound vibration or gentle probing. Test design: Five organisms per beaker, two beakers per concentration, at least 5 concentrations of ethanol.

	Method of calculating mean measured concentration: Not described. Nominal concentration: Range from 1 % v/v to 1.5% v/v according to graph. Measured concentration: Not measured. Statistical method: Probit.
Result	LC50 quoted as 1.28% v/v (1.18 to 1.38) which is equivalent to 10.1 (9,3 to 10.9) g/l. Control response not known.
Reliability	(2) valid with restrictions
Reference	Bowman, M., Oller, Wi, Cairns, T. (1981). Stressed bioassay systems foir rapid screening of pesticide residues. Part 1: Evaluation of bioassay systems. Arch. Environ. Contam. Toxicol. 10: 9-24.
11.11.2004	(90)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	Daphnia pulex (Crustacea)
Exposure period	18 hour(s)
Unit	g/l
EC50	= 12.1 measured/nominal
Analytical monitoring	No
Method	
Year	1981
GLP	no data
Test substance	ethanol (64-17-5)
Method	Organisms exposed to 4 concentrations of ethanol in the range 1% v/v to 2% vlv. Test conducted at 23 degC.
Remark	Biological observations: Number immobilized as compared to number exposed; mortality ranged from 0 to 100%. Concentration response with 95% confidence limits (LC50) 1.53% vlv (1.17-1.80). Cumulative immobilization: Not discussed. Satisfactory control response?: Unknown. Test organism: Daphnia pulex caught from a nearby pond. Age: less than 24 h old when used. Control group: None mentioned. Test conditions: Stock solutions preparation not discussed. Test temperature range 23 deg C +/- 1 deg. Exposure vessel: 50 ml culture tubes containing 25 ml test medium. Tubes loosely capped, not aerated. Each dilution tested in duplicate. Dilution water chemistry: Not measured.

	Lighting: 1 h of typical fluorescent light illumination, 15.5 h 10% normal illumination then 1.5 h typical illumination. Water chemistry on test: Not measured. Endpoint assessment: Organisms considered dead if they did not move after being swirled under a light. Test design: Ten organisms per tube, two tubes per concentration, at least 4 concentrations of ethanol. Method of calculating mean measured concentration: Not described. Nominal concentration: Range from 1 % v/v to 2% v/v according to graph. Measured concentration: Not measured. Statistical method: Probit.
Result	LC50 reported as 1.53% v/v (1.17 to 1.80) which is equivalent to 12.1 (9.2 to 14.2) g/1. Control response not known.
Test substance	USP grade, 95% ethanol
Reliability	(2) valid with restrictions
Reference	Bowman, M., Oller, Wi, Cairns, T. (1981). Stressed bioassay systems foir rapid screening of pesticide residues. Part 1: Evaluation of bioassay systems. Arch. Environ. Contam. Toxicol. 10: 9-24.
11.11.2004	(90)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	Artemia salina (Crustacea)
Exposure period	1 day(s)
Unit	mg/l
EC50	= 23874
Analytical monitoring	no data
Method	other: Artoxkit M
Year	1992
GLP	no data
Test substance	ethanol (64-17-5)
Method	This test used the Standard Operating Procedures for the ARTOXKIT M test modified as follows: The procedures of Vanhaecke (1980) and Vanhaeck & Persoone (1981) were followed for the hatching of the cysts and collection of the nauplii. For moulting of instar I to instar II-III larvae the nauplii were transferred after 18-24 h from the start of cyst rehydration to 100 mi Erlenmeyer flasks containing fresh artificial seawater with continuous aeration and illumination for a further 24 hr.

	LC50s were calculated with the corresponding 95% confidence limits using the trimmed Spearman Karber method. Control: Sodium dodecyl sulphate. An artificial seawater (35 g/l salt) was used: NaCI 23.9 g/l MgC12.6H2O 10.83 g/l CaCl2 1.15 g/l SrCI2.6H2O 4 mg/l KCI 682 mg/l KBr 9.9 mg/l Na2SO4 9.06 mg/l NaHCO3 200 mg/l NaF 0.3 mg/l H3BO3 2.7 mg/l
Result	The EC50 for artemia was 519 mmol/l +1- 29.1 (23.874g/l +1-1.33).
Test substance	analytical grade from Sigma Chemical Company.
Reliability	(2) valid with restrictions
Reference	Calleja, M.C., Persoone, G. Cyst based Toxicity Tests. IV. The potential of ecotoxicological tests for the prediction of acute toxicity in man as evaluated on the first ten chemicals of the MEIC programme. ATLA 20:396-405. Calleja. M.C., Persoone, G., Geladi, P. Comparative acute toxicity of the firt 50 multicentre evaluation of in vitro cytotoxicity chemicals in aquatic non-vertebrates. Arch Environ Contam Toxicol 1994; 26(1): 69-78.
11.11.2004	(91) (92)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	Daphnia magna (Crustacea)
Exposure period	1 day(s)
Unit	g/l
EC50	10.7 measured/nominal
Analytical monitoring	no data
Method	OECD Guide-line 202
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Method	1984 version of OECD method. 3 replicates. Statistics: trimmed Spearman-Karber method. No further data given.

Resul	Result quoted as 233mmol/1. No confidence limits given. No specific data.
Test substance	At least 97% pure, but possibly >99% or pharmacopia purity.
Reliability	(4) not assignable
Reference	Calleja, M.C., Persoone, G., Geladi, P. Comparative acute toxicity of the first 50 multicentre evaluation of in vitro cytotoxicity chemicals in aquatic non-vertebrates. Arch Environ Contam Toxicol 1994; 26(1): 69-78.
11.11.2004	(92)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	other: Brachionus calyciflorus
Exposure period	1 day(s)
Unit	g/l
LC50	29.6 measured/nominal
Analytical monitoring	no data
Method	other: Rotoxkit F
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Method	This test used the Standard Operating Procedures for the ROTOXKIT F test modified as follows: The contents of a vial containing B. calyciflorus cysts was emptied into a small disposable polystyrene Petri dish. 5 ml of EPA water was then added after which the whole was covered and incubated at 25C +/-1 in light (19.5uE.m-2) for 18-20hrs. 24 well plates used. LC50s were calculated with the corresponding 95% confidence limits using the trimmed Spearman Karber method. Control: Potassium dichromate EPA water < 2 weeks old and continuously aerated. KCI 4mg/l NaHCO3 296 g/l MgSO4 60 mg/l CaSO4.2H2O 60 mg/l
Result	Result quoted as 644mmol/l (+1-40.6) which is equivalent to 29.6g/1 (+1-1.9).
Test substance	analytical grade from Sigma Chemical Company.

Reliability	(2) valid with restrictions
Reference	Calleja, M.C., Persoone, G. Cyst based Toxicity Tests. IV. The potential of ecotoxicological tests for the prediction of acute toxicity in man as evaluated on the first ten chemicals of the MEIC programme. ATLA 20:396-405. Calleja, M.C., Persoone, G., Geladi, P. Comparative acute toxicity of the firt 50 multicentre evaluation of in vitro cytotoxicity chemicals in aquatic non-vertebrates. Arch Environ Contam ToxicoI1994;26(1):69-78.
11.11.2004	(91) (92)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	other: Brachionus plicatilis
Exposure period	1 day(s)
Unit	g/l
LC50	= 35.4 measured/nominal
Analytical monitoring	no data
Method	other: Rotox M
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Method	This test used the Standard Operating Procedures for the ROTOXKIT M test modified as follows: The contents of a vial containing B. plicatilis cystes , suspended in a saline medium of SSg/l, were poured into a small disposable polystyrene Petri dish. 5ml of deionised water was added to bring the salinity of the hatching medium to 15g/1. The whole was incubated at 25C+/-1 in light (19.5uE.m-2) for 24-28 hours. 24 well plates used. LC50s were calculated with the corresponding 95% confidence limits using the trimmed Spearman Karber method. Control: Cupric sulphate. An artificial seawater (15g/1 salt) was used: NaCI11.32g!1 MgC12.6H20 1.97g/1 CaCI2 0.54g/1 KCI 0.36mg/1 MgS04.7H20 2.39g/1 NaHC03 70mg/1 H3B03 10mg/1
Result	Quoted LC50 was 770 mmol/l (+/- 34.5) which is equivalent to 35.4 (+/-1.6) g/1.

Test substance	analytical grade from Sigma Chemical Company.
Reliability	(2) valid with restrictions
Reference	Calleja, M.C., Persoone, G. Cyst based Toxicity Tests. IV. The potential of ecotoxicological tests for the prediction of acute toxicity in man as evaluated on the first ten chemicals of the MEIC programme. ATLA 20:396-405. Calleja, M.C., Persoone, G., Geladi, P.. Comparative acute toxicity of the firt 50 multicentre evaluation of in vitro cytotoxicity chemicals in aquatic non-vertebrates. Arch Environ Contam Toxicol 1994;26(1):69-78.
11.11.2004	(91) (92)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Static
Species	other: Streptocephalus proboscideus
Exposure period	1 day(s)
Unit	g/l
LC50	= 18.8 measured/nominal
Analytical monitoring	no data
Method	other: Streptox F
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Method	This test used the Standard Operating Procedures for the STREPTOXKIT F test modified as follows: Hatching of the cysts was initiated 24hrs before the start of the test, in cylindrico-conical tube containing 100-125ml of EPA water at 25C +/-1 in light (19.5uE.m-2) and aerated. As described by Centeno (1992) hatched larvae (intstar I) were tranferred afte 16-18hrs from the start of the rehydration into Erlenmeyer flasks containing fresh medium and incubated for a further 5-7hrs to moult to the intart II-III stage. Control: Potassium dichromate LC50s were calculated with the corresponding 95% confidence limits using the trimmed Spearman Karber method. EPA water «2 weeks old and continuously aerated): KCl 4mg/1 NaHCO3 296 g/1

	MgSO4 60mg/l
Result	CaSO4.2H2O 60mg/l Quoted LC50 of 409mmol/l (+/- 12.9) which is equivalent to 18.8g/l (+/0.6).
Test substance	analytical grade from Sigma Chemical Company.
Reliability	(2) valid with restrictions
Reference	Calleja, M.C., Persoone, G. Cyst based Toxicity Tests. IV. The potential of ecotoxicological tests for the prediction of acute toxicity in man as evaluated on the first ten chemicals of the MEIC programme. ATLA 20:396-405. Calleja, M.C., Persoone, G., Geladi, P. Comparative acute toxicity of the firt 50 multicentre evaluation of in vitro cytotoxicity chemicals in aquatic non-vertebrates. Arch Environ Contam ToxicoI1994;26(1):69-78.
11.11.2004	(91) (92)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Other
Species	
Exposure period	1 day(s)
Unit	mg/l
IC50	= 13100 ~ 20900
Analytical monitoring	no data
Method	other
Year	1995
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	IC50 is for population growth in this freshwater protozoan, Tetrahymena pyriformis (Ciliata).
Result	Three incubation periods were evaluated with the following results: 3 hour 20900 mg/l 6 hour 17700 mg/l 9 hour 13100 mg/l
Reliability	(4) not assignable
Reference	Sauvant, M.P., Pepin, D., Groliere, CA, Bohatier, J. Effects of organic and inorganic substances on the cell proliferation of L-929 fibroblasts and Tetrahymena pyriformis GL Protozoa used for toxicological bioassays. Bull Environ Contam Toxicol 1995; 55(2):171-178.
21.08.2003	(93)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Other
Species	
Exposure period	1 day(s)
Unit	mmol/l
EC50	= 258
LC50	= 590
Analytical monitoring	no data
Method	other
Year	1999
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	EC50 values are for development in the protozoan Spirostomum ambiguum.
Reliability	(4) not assignable
Reference	Nalecz-Jawecki, G., Sawicki, J. Sirotox - A new tool for testing the toxicity of volatile compounds. Chemosphere 1999; 38(14): 3211-3218.
21.08.2003	(94)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	other
Species	aquatic crustacea
Exposure period	1 day(s)
Unit	mg/l
LC50	31700
Analytical monitoring	no data
Method	other
Year	1994
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	The species used was the Fairy shrimp, Streptocephalus rubricaudatus.
Reliability	(4) not assignable
Reference	Crisnel, A., Delaunay, L, Rossel, D., et al. Cyst-based ecotoxicological tests using Anastrocans: Comparison of two species of Streptocephalus. Environ Taxieol Water Qual 1994: 9(4): 317-326.
21.08.2003	(95)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Static
Species	Palaemonetes pugio (Crustacea)
Exposure period	4 day(s)
Unit	g/l
EC50	= 12.07 measured/nominal
Analytical monitoring	no data
Method	other
Year	1997
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Age at start: Adult male and female grass shrimps from local estuaries, Gulf Breeze, Fla, USA. Acclimation: to 25 Cel and 20 ppt salinity for 2 weeks. Embryos: Collected for test at embryo cap stage. Ethanol dosage: increasing concentrations (range not given} Duration of exposure: 12 days Mortality and hatching recorded daily.
Result	Mean LC50 at 4 days: 12.07 g/l Mean LC50 at 12 days: 3.63 g/l
Conclusion	If ethanol is used as a solvent in this developmental toxicity test it should not exceed 1 g/l in the test solution.
Reliability	(4) not assignable
Reference	Rayburn, J.R., Fisher, W.S. (1997). Developmental toxicity of three carrier solvents using embryos of the grass shrimp, Palaemonetes pugio. Arch Environ Contam Toxicol.
29.09.2003	33:217221. (96)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	
Species	Daphnia sp. (Crustacea)
Exposure period	1 day(s)
Unit	mg/l
EC50	= 12300 -13400
Analytical monitoring	no data
Method	other
Year	1996
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	The 2 day range was 10100 to 11200 mg/1.

Reliability	(4) not assignable
Reference	Rossini, G.D.S., Ronco, A.E. Acute toxicity bioassay using Daphnia obtusa as a test organism. Environ Toxicol Water Qual. 1996; 11 (3): 255-258.
21.08.2003	(97)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	
Species	Daphnia pulex (Crustacea)
Exposure period	1 day(s)
Unit	mmol/l
EC50	= 251.07
Analytical monitoring	no data
Method	other
Year	1995
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	
Reliability	(4) not assignable
Reference	Lilius, H., Hastbacka, T., Isomaa, B. A comparison of the toxicity of 30 reference chemicals to daphnia magna and Daphgnia pulex. Environ Toxicol Chem 1995;14(12): 2085-2088.
21.08.2003	(98)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	
Species	Daphnia magna (Crustacea)
Exposure period	24 hour(s)
Unit	mg/l
EC50	> 10000
Analytical monitoring	no data
Method	other
Year	1977
GLP	no data
Test substance	ethanol (64-17-5)
Result	Although the figure given in the paper is referred to as an LC50, it is better defined as an EC50, as the end-point studied is immobilization. Twenty-four-hour-old Daphnia exposed to a series of dilutions of ethanol in tap water. Swimming ability measured after 24 hours.

Reliability	(4) not assignable
Reference	Bringmann, G. & Kuhn, R. (1977) Befunde der Schadwirkung wassergefaehrdender Stoffe gegen Daphnia magna. Z. Wasser Abwasser Forsch.10, 161 -166.
11.11.2004	(99)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	
Species	Daphnia magna (Crustacea)
Exposure period	2 day(s)
Unit	g/l
LC100	1
Analytical monitoring	no data
Method	other
Year	1995
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Unit of concentration expressed as % (v/v or wlw not known).
Reliability	(4) not assignable
Reference	Baldwin, W.S., Milam. D.L. LeBlanc, GA Physiological and biological perturbations in Daphnia magna following exposure to the model environmental estrogen diethylstilboestrol. Environ T oxicol Chem 1995; 14(6):945-952. (100)
21.08.2003	

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Static
Species	Daphnia magna (Crustacea)
Exposure period	2 day(s)
Unit	g/l
EC50	> 100
Analytical monitoring	no data
Method	other
Year	1995
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Result is expressed in ppm.
Reliability	(4) not assignable
Reference	Office of Pesticide Programs. Environmental Effects Database(EEDB). Environmental Fate and Effects Division, U.S. EPA, Washington, D.C. 1995.

21.08.2003 (101)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	
Species	Daphnia magna (Crustacea)
Exposure period	1 day(s)
Unit	mg/l
EC50	> 10000
Analytical monitoring	no data
Method	other
Year	1989
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Same value recorded for 2 day exposure.
Reliability	(4) not assignable
Reference	Kuhn, R.T., Pattard, K., Pernak, K., Winter, A. Results of the harmful effects of selected water pollutants (anilines, phenols, aliphatic compounds) to Daphnia magna. Water Res. 1989; 23(4): 495-499.

21.08.2003 (102)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	
Species	Daphnia magna (Crustacea)
Exposure period	1 day(s)
Unit	mg/l
EC50	= 2500
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Effect is on physiology; EC50 (2 day) 2000 mg/l.
Reliability	(4) not assignable
Reference	Lagerspetz, K.Y.H., Tiiska, A.t Senius, KED. Low sensitivity of ciliary activity in the gills of Anodonta to some ecotoxicals. Camp Biochem Physiol 1993; 105(C3): 393-395.

21.08.2003 (103)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type

Species	Daphnia magna (Crustacea)
Exposure period	1 day(s)
Unit	mmol/l
EC50	= 297.7
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	
Reliability	(4) not assignable
Reference	Lilius, H., lsomaa, B., Holmstrom, T. A comparison of the toxicity of 50 reference chemicals to freshly isolated rainbow trout hepatocytes and Daphnia magna. Aquat Toxicol 1994; 30: 47-60.
21.08.2003	(104)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	
Species	Artemia sp. (Crustacea)
Exposure period	2 day(s)
Unit	mg/l
LC50	= 25500
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	
Reliability	(4) not assignable
Reference	Wu, Z., Chen, G. Studies of acute intoxication by some harmful substances on Penaeus orientalis K. Mar Sci/Haiyang Kexue 1988; 4: 36-40.
21.08.2003	(105)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	
Species	Artemia sp. (Crustacea)
Exposure period	1 day(s)
Unit	mg/l
LC50	= 25500 - 27000 measured/nominal
Analytical monitoring	no data
Method	other
Year	

GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	
Reliability	(4) not assignable
Reference	Wu, Z., Chen, G. Studies of acute intoxication by some harmful substances on Penaeus oriental is K. Mar Sci/Haiyang Kexue 1988; 4: 36-40.
21.08.2003	(105)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Static
Species	Artemia salina (Crustacea)
Exposure period	24 hour(s)
Unit	mg/l
TLm	> 10000
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Static test carried out in the laboratory at 24.5 C. TLm (concentration causing 50% mortality) determined graphicallyfrom measurements at an unspecified number of concentrations.
Reliability	(4) not assignable
Reference	Price, K.S. et at (1974) Brine shrimp bioassay and seawaterBOD of petrochemicals. J. Water Pollut. Control Fed. 46/63 - 77.
21.08.2003	(106)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	
Species	Other
Exposure period	2 day(s)
Unit	mg/l
EC50	= 11963
Analytical monitoring	no data
Method	other
Year	1990
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Endpoint is EC50 for growth in the freshwater protozoan

	Tetrahymena pyriformis (Ciliata).
Reliability	(4) not assignable
Reference	Schultz, T.W., Arnold, L.M., Wilke, T.S., Moulton, M.P. Relationships of quantitative structure-activity for normal aliphatic alcohols. Ecoptoxicol Environ Saf 1990; 19(3): 243-253.
21.08.2003	(107)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	
Species	Other
Exposure period	2 day(s)
Unit	mmol/1
IC50	259.67
Analytical monitoring	no data
Method	other
Year	1993
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	IC50 is for population growth in this freshwater protozoan. Tetrahymena pyriformis (Ciliata).
Reliability	(4) not assignable
Reference	Schultz, T.W., Tichy, M. Structure-toxicity relationships for unsaturated alcohols to Tetrahymena pyriformis: C5 and C6 analogs and primary propargylic alcohols. Bull Environ Contam Toxicol 1993; 51(5): 681-688.
21.08.2003	(108)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Preferred method	
Test Substance:	n-Butyl Alcohol
Method:	OECD 202, USEP A TSCA 40 CFR 797.1300
Year (guideline):	1984, 1994
Type (test type):	Static Daphnid Acute Toxicity Test
GLP:	Yes
Year (study performed):	1998
Species:	Water flea (Daphnia magna)
Analytical Monitoring	Yes
Exposure Period:	48 Hours
Statistical Method:	(FT ME)* Binomial probability with non-linear interpolation
Test Conditions:	(FT - TC)
Note:	Test solutions were prepared by diluting a 50-mg/mL stock solution of n-butyl alcohol (99.9% purity) with moderately

hard, filtered [0.2 mm] well water to nominal concentrations of 156, 259,432, 720, 1200, and 2000 mg/L Stock solution was also prepared with well water. Test vessels were 250-mL beakers containing approximately 200 mL (7.8-cm depth) of test solution. Two replicate test vessels were maintained for each treatment and control (dilution water) group. Vessels were covered to prevent evaporation and placed in a water bath at 20±l degree C with a 16-hour light: 8-hour dark photoperiod (391 lux).

Water samples for analytical verification were collected from each replicate of the control and treatments at test initiation and termination.

Dissolved oxygen exceeded 60% saturation and pH ranged from 8.2 to 8.5. Temperature ranged from 19.4 to 19.7 dc. Dilution water total organic carbon was <1 mg C/L. Total hardness, alkalinity, and specific conductance of dilution water were 128 mg/L as CaCO3, 180 mg/L as CaCO3, and 300 mmhos/cm, respectively.

Daphnids were obtained from in-house cultures. Adult organisms were held for at least 16 days prior to collection of neonates for testing. Twenty daphnids (10 per replicate) <24 hours old were exposed to each test concentration and control (dilution water).

Results: (FT - RS) 48-hour EC50 was 1328 mg/L (95% CL: 1123 and 1925 mg/L) based on mean measured concentrations.

Some organisms appeared lethargic in the 675 mg/L test solution after 48 hours and in the 1123 mg/L treatment after 21, 24, and 48 hours. All surviving organisms exposed to 1925 mg/L appeared lethargic at the 21 and 24-hour observations.

Reliability: (1) valid without restriction

Reference: Wong, D.C.L, P.B. Dom, and J.P. Sa1anitro. 1998. Aquatic Toxicity of Four Oxy-So1vents. Equilon Enterprises, LLC Technical Information Record WTC-3520.

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Test substance: 1-Butanol

Test species: Water flea (Daphnia magna)

Test method: Not Stated

GLP: No

Test results: 48 Hr. EC50 2337 mg/L
48 Hr. EC50 1983 mg/L
Reliability: (2) valid with restrictions, full experimental data not presented
Reference: Kuehn, R., M. Pattard, K.D. Pernak, and A. Winter. (1989). Results of the Harmful Effects of Water Pollutants to Daphnia Magna in the 21 Day Reproduction Test. Water Res 23(4): 495-499.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-butanol (71-36-3)
Value: 615 mg/L
Remark: An acute daphnid 48-h LC50 was calculated using ECOSAR, from the U.S. EP A. The preferred physical properties were used. The SAR for esters was employed. The structure was determined from the CAS RN as stored in the accompanying database of SMILES notations within ECOSAR. Chemicalspecific input parameters were: molecular weight (74.12 g/mol), vapor pressure (0.56 hPa or 0.42 mm Hg), log Kow (0.88), melting point -89.90 C, aqueous solubility 77,000 mg/L, boiling point of 117.6° C, and a Henry's Law constant of 5.3 E7 atm-m3/mol.
(2) valid with restriction, calculated value
Reliability: EPA's ECOSAR model (v. O.99f). EPISUITE v.3.10, U.S.
Reference: Environmental Protection Agency, April (2001).

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l
Analytical monitoring: no
EC0: = 152
EC50: = 201
EC100: = 270
Limit Test: no

Method: other
Year: 1982
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Result: RESULTS: EXPOSED
EC0: 152 mg/l

EC50: 201 mg/l
E100: 270 mg/l
Based on nominal concentration
RESULTS: CONTROL
Number/% showing adverse effects: Not reported

Test condition: TEST ORGANISMS
Strain: Daphnia magna
Supplier: Laboratory culture
Age: <24hrs old
Feeding: Dry algae
Pretreatment: None
Feeding during test: Not reported
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF THE TEST CHEMICAL SOLUTIONS: no analysis
DILUTION WATER
Source: Standardised synthetic fresh water
Aeration: None
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: Range of test concentrations to achieve three or more responses between 0 and 100%
Renewal of test solution: none
Exposure vessel type: 50 ml flask
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 20 C
Dissolved oxygen: oxygen saturated
pH mean: 7.6 - 7.7
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: 9 hours artificial lighting
TEST PARAMETER: Mortality/immobility

MONITORING OF TEST SUBSTANCE CONCENTRATION:
None

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Bringmann, V. and Kuhn, R. 1982. Results of toxic action of water pollutants on Daphnia magna Straus tested by an improved standardized procedure. Z. Wasser Abwasser Forsch. 15(1):1-6.

21-JUL-2005 (15)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: static
Species: Nitocra spinipes (Crustacea)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no data
LC50 : = 317
Limit Test: no

Method: other
Year: 1984
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Method: The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Twenty invertebrates were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
Remark: This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity and with standard test organisms are available
Reference: Bengtsson, B., Renberg, L., and Tarkpea, M. 1984. Molecular structure and aquatic toxicity-An example with C1-C13 aliphatic alcohols. Chemosphere 13(5/6):613-622.

Linden, E., Bengtsson, B.E., Svanberg, O., and Sundstrom, G. 1979. The acute toxicity of 78 chemicals and pesticide formulations against two brackish water organisms. The bleak (Alburnus alburnus) and the harpaticoid Nitocra spinipes. Chemosphere 11-12:843-851.
19-JUL-2005 (9) (34)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: static
Species: other: tubifex tubifex (Oligochaeta)
Exposure period: 3 minute(s)
Unit: mg/l

Analytical monitoring:
EC50: = 110
Limit Test: no

Method: other
Year: 1997
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Method: Test media were prepared by dilution of a stock solution. The acute immobilisation test was carried out under static conditions. The EC50 was based on counting the number of worms that stopped moving within 3 minutes of exposure to test medium.
Reliability: (4) not assignable
Documentation insufficient for assessment. Information obtained from the open literature. Only a brief description of the test method is given.
Reference: Rucki, M. and Tichy, M. (1997). Acute toxicity of alcohols: Prediction by QSAR analysis and molecular similarity. Centr. Eur. J. publ. Hlth 5, No.4, p. 183-187.
20-OCT-2005 (56)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Unit: mg/l
Analytical monitoring: no
EC50: = 123.6 calculated

Method: other
Year: 2005
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (2)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC0: = 6.8
EC50: = 20
EC100: = 71
Limit Test: no

Method: other:
Year: 1982
GLP: no
Test substance: > 90% 1-octanol (111-87-5)

Result: RESULTS: EXPOSED
EC0: 6.8 mg/l
EC50: 20 (15-26) mg/l
E100: 71 mg/l
Based on nominal concentration
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
Test condition: TEST ORGANISMS
Strain: Daphnia magna
Supplier: Laboratory culture
Age: <24hrs old
Feeding: Dry algae
Pretreatment: None
Feeding during test: Not reported
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF THE TEST CHEMICAL SOLUTIONS: no analysis
DILUTION WATER
Source: Standardised synthetic fresh water
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported

Conductance: Not reported
TEST SYSTEM
Concentrations: Range of test concentrations to achieve three or more responses between 0 and 100%
Renewal of test solution: none
Exposure vessel type: 50 ml flask
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 20 C
Dissolved oxygen: oxygen saturated
pH mean: 7.6 - 7.7
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: 9 hours artificial lighting
TEST PARAMETER: Mortality/immobility
MONITORING OF TEST SUBSTANCE CONCENTRATION: None

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Bringmann, V. and Kuhn, R. 1982. Results of toxic action of water pollutants on Daphnia magna Straus tested by an improved standardized procedure. Z. Wasser Abwasser Forsch. 15(1):1-6.

19-JUL-2005 (28)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC0: = 19
EC50: = 26
Limit Test: no

Method: other
Year: 1989
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Remark: This acute 24 hour daphnia test was carried out prior to a 21 day reproduction test in daphnia. No information is given on the test conditions.
The nominal concentrations were given as no results of chemical analysis were available for the 24 hour EC50.

Reliability: (2) valid with restrictions

Not key study: Other studies (same reliability scores) but with higher toxicity values are available.

Reference: Kuhn, R. and Pattard, M. 1990. Results of the harmful effects of water pollutants to green algae (Scenedesmus subspicatus) in the cell multiplication inhibition test. Wat. Res. 24(1):31-38.

19-JUL-2005 (74)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: static
Species: Nitocra spinipes (Crustacea)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC50 : = 58
Limit Test: no

Method: other
Year: 1984
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Method: The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Twenty invertebrates were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.

Remark: This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity and with standard test organisms are available

Reference: Bengtsson, B., Renberg, L., and Tarkpea, M. 1984. Molecular structure and aquatic toxicity-An example with C1-C13 aliphatic alcohols. Chemosphere 13(5/6):613-622.

Linden, E., Bengtsson, B.E., Svanberg, O., and Sundstrom, G. 1979. The acute toxicity of 78 chemicals and pesticide formulations against two brackish water organisms. The bleak (Alburnus alburnus) and the harpaticoid Nitocra spinipes. Chemosphere 11-12:843-851.

19-JUL-2005 (19) (77)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Species: Daphnia magna (Crustacea)
Unit: mg/l
Analytical monitoring: no data
LC50 : = 36.6
Limit Test: no

Method: other: standard
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Remark: The LC50 reported here (36.6 mg/L) reflects a mean of two other studies; 47 mg/L reported in Bringmann and Kuhn 1977 and 26 mg/L reported in Burton 1992. Bringmann and Kuhn 1977 study was superceded by Bringmann and Kuhn 1982 which reported a lower EC50. The Burton 1992 study is not available.
Reliability: (4) not assignable
Not key study: This result is a secondary report from two previous studies.
Reference: Bringman, G. and Kuhn, R. 1977. Results of the damaging effect of water pollutants on Daphnia magna. Z. Wasser-Abwasser-Forsch 10:161-166.

Burton, W.D. 1992. An evaluation of aquatic toxicity data with a population growth model for application to environmental hazard assessment. Gov. Rep. Announce. 10:1-157.

Toussaint, M.W., Shedd, T.R., van der Schalie, W.H., and Leather, G.R. 1995. A comparison of standard acute toxicity tests with rapid-screening toxicity tests. Environmental Toxicology and Chemistry 14 (5): 907-915.
19-JUL-2005 (22) (33) (112)

<u>1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)</u>

Species: other: Ceriodaphnia dubia
Exposure period: 48 hour(s)
Unit: mg/l
Analytical monitoring:
EC50: = 8.7

Test substance: > 90% 1-octanol (111-87-5)

Reliability: (4) not assignable
Not key study. This result is a secondary report from Burton

1992 which is not available. No details are available.

Reference: Burton, W.D. 1992. An evaluation of aquatic toxicity data with a population growth model for application to environmental hazard assessment. Gov. Rep. Announce. 10:1-157.

Toussaint, M.W., Shedd, T.R., van der Schalie, W.H., and Leather, G.R. 1995. A comparison of standard acute toxicity tests with rapid-screening toxicity tests. Environmental Toxicology and Chemistry 14(5):907-915.

19-JUL-2005 (33) (112)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Species: Gammarus sp. (Crustacea)

Test substance: > 90% 1-octanol (111-87-5)

Result: 4 - 40 min EC50 = 6.3 - 7.2 mg/l

Reliability: (4) not assignable

Not key study: Other studies with higher reliability score are available

Reference: Verschueren, K. (ed.). 1996. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York: John Wiley & Sons, Inc.

19-JUL-2005 (122)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: static

Species: other: Tubifex tubifex (Oligochaeta)

Exposure period: 3 minute(s)

Unit: mg/l

Analytical monitoring: no data

EC50: = 190

Limit Test: no

Method: other

Year: 1997

GLP: no data

Test substance: > 90% 1-octanol (111-87-5)

Method: Test media were prepared by dilution of a stock solution. The acute immobilisation test was carried out under static conditions. The EC50 was based on counting the number of worms

that stopped moving within 3 minutes of exposure to test medium.

Reliability: (4) not assignable
Documentation insufficient for assessment. Information obtained from the open literature. Only a brief description of the test method is given.

Reference: Rucki, M. and Tichy, M. (1997). Acute toxicity of alcohols: Prediction by QSAR analysis and molecular similarity. Centr. Eur. J. publ. Hlth 5, No.4, p. 183-187

09-SEP-2005 (94)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Unit: mg/l
Analytical monitoring: no
EC50: = 25 calculated

Method: other
Year: 2005
GLP: no
Test substance: > 90% 1-octanol (111-87-5)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown.

Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

21-DEC-2005 (4)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: static
Species: Daphnia magna (Crustacea)

Exposure period: 48 hour(s)
Unit: mg/l
Analytical monitoring: no data
EC0: = .3
EC50: = 2.9
EC100: = 29
Limit Test: no

Method: other
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Method: German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on microcrustaceans (Daphnia Shorttime Test)(L11).
This method corresponds to the OECD Guideline 202, part 1.
Remark: Static exposures. Endpoint was immobilization. This information is from a 1 page summary of the full report which is not available but an OECD standard method was used. 20 animals per concentration.
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Henkel KGaA. 1999b. 1-Decanol: Acute toxicity: Daphnia. Biological Research and Safety/Ecology: Unpublished results; test substance registration No. 7843.
19-JUL-2005 (42)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Type: static
Species: Nitocra spinipes (Crustacea)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no data
LC50 : = 3.1
Limit Test: no

Method: other
Year: 1984
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Method: The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Twenty invertebrates were

exposed to each concentration. Water was maintained at pH 7.9 and 10 degree C.

Remark: This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity and with standard test organisms are available

Reference: Bengtsson, B., Renberg, L., and Tarkpea, M. 1984. Molecular structure and aquatic toxicity-An example with C1-C13 aliphatic alcohols. Chemosphere 13(5/6):613-622.

Linden, E., Bengtsson, B.E., Svanberg, O., and Sundstrom, G. 1979. The acute toxicity of 78 chemicals and pesticide formulations against two brackish water organisms. The bleak (Alburnus alburnus) and the harpaticoid Nitocra spinipes. Chemosphere 11-12:843-851.

19-JUL-2005 (15) (62)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Species: Daphnia magna (Crustacea)
Unit: mg/l
Analytical monitoring: no data
EC50: = 4.4

GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Remark: Indicated in table as unpublished results (S Marshall, Unilever Research). Test solutions were prepared using sonication but no solvents.

Reliability: (4) not assignable
Not key study: Other studies with higher reliability score are available, data obtained from secondary literature

Reference: Unilever. 1995. Bioavailability: Research Contract Sponsored by the Department of the Environment. Final Report. June 1995.

19-JUL-2005 (92)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)

Unit: mg/l
Analytical monitoring: no
NOEC: = 2.8
LC50 : = 6.5
Limit Test: no

Method: other: USEPA 1975.
Year: 1976
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)
Remark: Static bioassays were conducted using replicate vessels, which were maintained at 22 C. Five daphnids (less than 24 hours old) were randomly assigned to each test vessel within 30 minutes after ALFOL 10 was added for a total of 15 Daphnia per concentration. Five concentrations plus control were tested.
Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
Reference: E.G.& G. Bionomics. 1976. Acute toxicity of ALFOL 810 and ALFOL 10 alcohols to Daphnia magna. Bioassay report submitted to Continental Oil Company, Ponca City, Oklahoma.
05-OCT-2005 (25)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l
Analytical monitoring: no data
EC50: = 11
Limit Test: no

Method: other
Year: 1982
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Remark: Daphnids were 24 hours old to begin the test. Test medium was tap water free from chlorine, saturated with oxygen, hardness of 16, pH = 7.6 - 7.7, and temperature of 20-22 C.
Reliability: (4) not assignable
Reference: Bringmann, V. and Kuhn, R. 1982. Results of toxic action of water pollutants on Daphnia magna Straus tested by an improved standardized procedure. Z. Wasser Abwasser Forsch.

15 (1): 1-6.
20-OCT-2005 (18)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l
Analytical monitoring:
EC0: = 8.8
EC50: = 16
EC100: = 25

Method: other: static test
Test substance: > 90% 1-decanol (112-30-1)

Method: Test condition: 20-22 degr. C, pH 7.6-7.7, parameter: mobility, no aeration, stock solution of test substance in water until optically clear.
Source: Henkel KGaA Duesseldorf
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
Reference: IUCLID Data Set: 1-Decanol. Shell Chemicals Ltd. May 11, 2006.
20-OCT-2005

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Unit: mg/l
Analytical monitoring: no
EC50: = 2.1 calculated

Method: other
Year: 2005
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give

the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.
A key input to this model is the compositional breakdown.

Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

21-DEC-2005 (3)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l
Analytical monitoring: no
NOEC: = .316
EC50: = .765
EC100: = 1.78
Limit Test: no

Method: OECD Guide-line 202
Year: 1997
GLP: yes
Test substance: other TS: Dodecanol (112-53-8)

Remark: The test substance was water-insoluble, however, a fine-turbid suspension could be prepared using slightly prewarmed demineralised water (23 C to 25 C). The test substance and prewarmed water were placed into vessels and were shaken manually for 3 minutes. The resulting suspension remained stable even at temperatures of 20 C and could be diluted. The suspensions were not filtered. Note, effects seen at concentration less than SPARC estimated water solubility.
The tests reported in this entry used a standard methodology. An additional test was also carried out using a non-standard submergible chamber procedure. Test concentrations were 0.316, 0.562, 1.00, 1.78, 3.16 and 5.62 mg/l. The EC50 was determined to be 1.589 mg/l based on nominal concentrations.

Result: RESULTS: EXPOSED
EC0 = 0.316 mg/l
EC50 = 0.765 mg/l

EC100 = 1.78 mg/l
Based on nominal concentration
RESULTS: CONTROL
Number/% showing adverse effects: 0

Source: Laboratory of Pharmacology and Toxicology 1997.

Test condition: TEST ORGANISMS
Strain: Daphnia magna
Supplier: Institut fur Wasser-, Boden-, und Lufthygiene
Age: 6-24 hours old
Feeding: Algae and a small amount of aerated sewage
Pretreatment: None
Feeding during test: None
Control group: 1 control group (4 replicates)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: None
Concentration of vehicle, solvent: None
STABILITY OF TEST CHEMICAL SOLUTIONS
No analysis
DILUTION WATER
Source: Reconstituted, aerated, fully demineralised water
Aeration: Not reported
Alkalinity: 0.8 mmol/l
Hardness: 250 mg CaCO3/l
Conductance: Not reported
TEST SYSTEM
Concentrations: 0.178, 0.316, 0.562, 1.00, 1.78, and 3.16 mg/l
Renewal of test solution: None
Exposure vessel type: all glass vessels , diameter: 38 mm, height: 60 mm, volume: 50 ml
Number of replicates: 4
Invertebrate per replicate: 5
Test temperature: 20 C
Dissolved oxygen: >80% of maximum saturation
pH mean: 7.9
Adjustment of pH: None
Intensity of irradiation: Not reported
Photoperiod: 16 hours light/8 hours darkness
white type fluorescent light
TEST PARAMETER: Immobilization
MONITORING OF TEST SUBSTANCE CONCENTRATION: None

Reliability: (2) valid with restrictions

Flag: Critical study for SIDS endpoint

Reference: Laboratory of Pharmacology and Toxicology. 1997. Examination of 1-Dodecanol in an acute immobilization test in Daphnia magna. LPT Report No. 10762/97.

12-MAR-2004 (12)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)

Species: Daphnia magna (Crustacea)
Unit: mg/l **Analytical monitoring:** no data
EC50: = .45

GLP: no data
Test substance: other TS: Dodecanol (112-53-8)
Remark: Indicated in table as unpublished results (S Marshall, Unilever Research). Test solutions were prepared using sonication but no solvents.
Source: Unilever, 1995.
Reliability: (4) not assignable
Not key study: Other studies with higher reliability score are available, data obtained from secondary literature
Reference: Unilever. 1995. Bioavailability: Research Contract Sponsored by the Department of the Environment. Final Report. June 1995.

12-MAR-2004 (21)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)

Type: static
Species: Nitocra spinipes (Crustacea)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no data
EC50: = 1
Limit Test: no

Method: other
Year: 1984
GLP: no data
Test substance: other TS: Dodecanol (112-53-8)

Method: The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Twenty invertebrates were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
Remark: This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.

Source: Bengtsson, 1984
Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity but with standard test organisms are available
Reference: Bengtsson, B., Renberg, L., and Tarkpea, M. 1984. Molecular structure and aquatic toxicity-An example with C1-C13 aliphatic alcohols. Chemosphere 13(5/6):613-622.

Linden, E., Bengtsson, B.E., Svanberg, O., and Sundstrom, G. 1979. The acute toxicity of 78 chemicals and pesticide formulations against two brackish water organisms. The bleak (Alburnus alburnus) and the harpaticoid Nitocra spinipes. Chemosphere 11-12:843-851.
12-MAR-2004 (1) (14)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l
Analytical monitoring: no
EC0: = 100
EC50: = 320
EC100: = 1000
Limit Test: no

Method: other
GLP: no data
Test substance: other TS: Dodecanol (112-53-8)

Method: German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on microcrustaceans (Daphnia Shorttime Test)(L11).
This method corresponds to the OECD Guideline 202, part 1.
Source: Henkel KGaA 1999q
Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
Reference: Henkel KGaA. 1999q. Dodecanol: Acute toxicity Daphnia. Unpublished data, Test substance registration no. 910724.
12-MAR-2004 (11)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Species: Daphnia magna (Crustacea)
Unit: mg/l
Analytical monitoring: no data
EC50: = 4

GLP: no data
Test substance: > 95% 1-tetradecanol (112-72-1)

Remark: Indicated in table as unpublished results (S Marshall, Unilever Research). Test solutions were prepared using sonication but no solvents.
The absence of any measurements of dissolved concentration, at nominal loadings very much greater than the water solubility, suggests the possibility of an artefactual dose-response.
Source: Unilever. 1995.
Reliability: (4) not assignable
This is a key study as it is the only one available for effects of C14 on invertebrates. However, no details are available and data obtained from secondary literature.
Flag: Critical study for SIDS endpoint
Reference: Unilever. 1995. Bioavailability: Research Contract Sponsored by the Department of the Environment. Final Report. June 1995.
19-OCT-2005 (75)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Unit: mg/l
Analytical monitoring: no
EC50: = .18 calculated

Method: other
Year: 2005
GLP: no
Test substance: > 95% 1-tetradecanol (112-72-1)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (4)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Unit: mg/l
Analytical monitoring: no
EC50: > 100 calculated

Method: other
Year: 2005
GLP: no
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.
A key input to this model is the compositional breakdown.
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
Flag: Critical study for SIDS endpoint
Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (4)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l

Analytical monitoring: no data
EC0: = 1000
EC50: = 1700
EC100: = 3000
Limit Test: no

Method: other: German Industry Standard DIN 38412, Part 11
Year: 1992
GLP: yes
Test substance: other TS: Octadecanol (112-92-5)

Method: METHOD FOLLOWED: German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on microcrustaceans (Daphnia Shorttime Test)(L11). DIN 38412, Part 11.
This method corresponds to the OECD Guideline 202, part 1.
DEVIATIONS FROM GUIDELINE: not reported
STATISTICAL METHODS: not reported
METHOD OF CALCULATION: EC50 was calculated according to Stephan (square root of EC0 * EC100)
Remark: The solubility of C18 alcohol (Octadecanol) is about 0.001 mg/l, therefore the LC50 was not achieved at the solubility limit.
Result: RESULTS: EXPOSED
Nominal/measured concentrations: nominal
Effect data (Immobilisation): up to loadings of 1000 mg/l no immobilisation, at 3000 mg/l and 10000 mg/l 100% immobilisation
Effect concentration vs. test substance solubility: nominal loadings were well in excess of water solubility
RESULTS CONTROL: <10% mortality
Source: Guhl 1992e.
Test condition: TEST ORGANISMS
Strain: Daphnia magna
Supplier: own breed
Breeding method: not reported
Age: not reported
Feeding: green algae (Chlorella kessleri)
Pretreatment: not reported
Feeding during test: No
Control group: yes
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: none
Vehicle, solvent: none
Other procedures: test substance was directly weighed into

the test vessels
STABILITY OF THE TEST CHEMICAL SOLUTIONS: Dissolved Oxygen Concentration (DOC) was measured for test substance concentrations of 1000 and 10000 mg/l and varied during the test between 0.3 and 0.5 mg/l (1000 mg/l) and 0.5-0.8 mg/l (10000 mg/l).
REFERENCE SUBSTANCE: not reported
DILUTION WATER:
Source: synthetic water according to DIN 38412, Part 11
TEST SYSTEM
Concentrations: 0, 10, 30, 100, 300 and 1000 mg/L
Renewal of test solution: No
Exposure vessel type: not reported
Number of replicates: not reported
Invertebrate per replicate: not reported
Test temperature: 20-21 C
Dissolved oxygen: 90-100% saturation
pH mean: 7.9-8.1
Adjustment of pH: not reported
DURATION OF THE TEST: 48 hours
TEST PARAMETER: Immbolization

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Guhl Dr. 1992e. 1-Octadecanol: Acute toxicity: Daphnia. Biological Research and Safety/Ecology: Unpublished results; test substance registration No. 910722; Henkel KGaA; Report No. RE 920020; (with English summary Report No. R9901352).
12-MAR-2004 (3)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Unit: mg/l **Analytical monitoring:** no
EC50: > 100 calculated

Method: other
Year: 2005
GLP: no
Test substance: >= 90% 1-eicosanol (629-96-9)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are

summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

Result: Predicted to be non-toxic at the limit of solubility.

Reliability: (2) valid with restrictions

The value was predicted using a multiple partitioning model, supported by additional validation.

Flag: Critical study for SIDS endpoint

Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

21-DEC-2005 (2)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Unit: mg/l **Analytical monitoring:** no

EC50: > 100

Method: other

Year: 2005

GLP: no

Test substance: >95% 1-docosanol (661-19-8)

Method: For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

Result: Predicted to be non-toxic at the limit of solubility.

Reliability: (2) valid with restrictions

The value was predicted using a multiple partitioning model, supported by additional validation.

Flag: Critical study for SIDS endpoint

Reference: Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

21-DEC-2005 (2)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Unit: mg/l
Analytical monitoring: no
LC50: = 3.71×10^{-6} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-tetracosanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, (2006).
05-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Unit: mg/l
Analytical monitoring: no
LC50: = 5.03×10^{-7} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-hexacosanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, (2006).
05-APR-2007

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Unit: mg/l
Analytical monitoring: no
LC50: = 6.92×10^{-8} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-octacosanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, (2006).
05-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Unit: mg/l **Analytical monitoring:** no
LC50: = 9.49×10^{-9} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-triacontanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, (2006).
05-APR-2007

4.3 Toxicity to Aquatic Plants e.g. Algae

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Chlorella vulgaris (Algae)
Endpoint	growth rate
Exposure period	4 day(s)
Unit	mg/l
NOEC	< 500 measured/nominal
LOEC	= 500 measured/nominal
EC50	= 1000 measured/nominal
Limit test	
Analytical monitoring	No
Method	other
Year	1996
GLP	no data
Test substance	no data
Method	Growth rate measured as chlorophyll content and biomass accumulation at concentrations of 0.05% (500 mg/l) and higher (range 500 to 10,000 mg/l). Cells removed before measurement: cells were not removed.

Remark

Biological observations:
+Cell density at each flask/each measuring point: Not given.
+Growth curves: Chlorophyll content plotted over time for each concentration, including control.

Percent biomass/growth rate inhibition per concentration
Observations at 500, 1000,2000,5000 and 10,000 mg/l, the growth inhibition was 37%, 54%, 69%, 86% and 95%
Laboratory culture: isolated from lake Geneva in 1980.

Cultivation method: Cultures were grown in Algal Assay Procedure (1971) medium in 500 ml flasks containing 250 ml algal suspension.

Cells were not removed from medium prior to measurement; cell density not given.

Controls consisted of algal suspensions without solvent in each experiment.

Dilution water source not specified.

Growth/test medium: Algal assay Procedure (1971) medium with 15 mg/I NaHC03 and 12 mgll K2HP04.

Exposure vessel type: 20 x 125 mm test tubes containing about 20 ml of suspension and ethanol. 3 Tubes per test concentration were used.

Water chemistry (pH) on test: Not described.

Stock solution preparation: Not described.

Light levels and quality during exposure: 100 microElmA2-sec except when reduced to 1.5 microElmA2-sec 20 min before and during measurement of chlorophyll content by fluorescence.

Test design: Ethanol was tested three times at each concentration (0, 0.05, 0.1, 0.3, 0.5 and 1 %).

Method of calculating mean measured concentrations: Only nominal concentrations were used.

Result

Growth was inhibited 54% at an ethanol concentration of 1000 mg/I, the value approximating the EC50.

	Growth inhibition was 37% at 500 mg/1. Growth was significantly inhibited (p=0.05) at all concentrations of ethanol.
Test condition	Test temperature 21 +/-1 deg C with continuous illumination at 100 microE/m^2-sec.
Conclusion	Growth was inhibited 48% at an ethanol concentration of 10,000 mg/I; this approximates the ErC50.
Reliability	(1) valid without restriction
Flag	Critical study for SIDS endpoint
Reference	El Jay, A. (1996) Toxic effects of organic solvents on the growth of Chiarella vulgaris and Selenastrum capricornutum. Bull. Environ. Contam. Toxicol. 57:191-198.
11.11.2004	(109)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	other aquatic plant: Lemna gibba
Endpoint	growth rate
Exposure period	7 day(s)
Unit	mg/l
NOEC	= 280 measured/nominal
LOEC	> 280 measured/nominal
EC50	= 4432 measured/nominal
Limit test	
Analytical monitoring	No
Method	EPA OTS 797.1160
Year	1986
GLP	no data
Test substance	ethanol (64-17-5)
Method	Lemna gibba (Fat Duckweed) was exposed to alcohol in water at nominal concentrations 0,1.0,1.7,2.8,4.7,7.8,13, 21,36 etc to 21,000 (21 concentrations) for 7 days. Maintained at 25 degC with 6461 +/- 323 lux continuously; 5382 +/- 89 on test. Grown on Hoagland's with a pH of 4.6 to 5.4. Medium renewed weekly. Acclimation period was 8 weeks.
Remark	Cells removed before measurement: Plant fronds counted visually. Biomass measured by dry weight of plants and fronds Biological observations: +Cell density at each flask/each measuring point: Not applicable. +Growth curves: Not shown.

Percent biomass/growth rate inhibition per concentration
Observations: Results were not given for each of the 21 occurrences. % EPA procedures as described by Holst (1986) and Holst and Edwanger (1982).
Laboratory culture: Obtained from Smithsonian Institution.

Cultivation method: Cultures were grown in Hoaglands medium with pH 4.6 to 5.4 medium was renewed weekly.

Acclimation period was 8 weeks.

Plants were not removed from medium prior to measurement; Plant density not given.

Controls consisted of Lemna cultures without ethanol in each experiment.

Dilution water source not specified.

Growthltest medium chemistry: Hoaglands. Water hardness 636 mgll as CaCO3; Alkalinity 23 mgll as CaCO3, Conductivity 5000 micromhos/cm, pH 4.5 to 5.1.

Exposure vessel type: 250 ml vessels; Shimadzu closures covered with paraffin. Each concentration replicated 3 times

Water chemistry (pH) on test: pH ranged 4.6 to 5.1..

Stock solution preparation: Not described.

Light levels and quality during exposure: Mean lux 5382 +/89 during exposure.

Result

Test design: Ethanol was tested three times at each concentration (1.0 to 21,000 mg/l, plus control). Only nominal concentrations were used.

Method of calculating mean measured concentrations: Only nominal concentrations were used.

Statistical method: EC50 - regression analysis; NOEL: Dunnett's test.

Test condition

The EC50 (4432 mg/l) was within the 95% confidence interval 845 to 8018 mg/l for plant growth. The EC50 for biomass (dry weight) was 5987 mg/l (1640 to 10,293) mg/J.

Conclusion	Ethanol was the least toxic of 8 compounds tested.
Reliability	(1) valid without restriction
Reference	Cowgill, U., Milazzo, D., Landenberger, B. (1991). The senisitivity of Lemna gibba G-3 and four clones of Lemna minor to eight common chemicals using a 7-day test, Res. J. Water Pollut. Control Fed. 63:991-998.
11.11.2004	(110)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	other aquatic plant Lemna minor 6591
Endpoint	growth rate
Exposure period	7 day(s)
Unit	mg/l
NOEC	= 778 measured/nominal
LOEC	> 778 measured/nominal
EC50	= 3690 measured/nominal
Limit test	
Analytical monitoring	No
Method	EPA OTS 797.1160
Year	1986
GLP	no data
Test substance	other TS: 100% dehydrated ethanol (64-17-5)
Method	Lemna minor (duckweed) was exposed to alcohol in water at nominal concentrations 0, 1.0,1.7,2.8,4.7,7.8,13,21, 36 etc to 21,000 for 7 days. Maintained at 25 degC with 6461 +/- 323 lux continuously; 5382 +/- 89 on test. Grown on Hoagland's with a pH of 4.6 to 5.4. Medium renewed weekly. Acclimation period was 8 weeks.
Remark	EPA procedures as described by Holst (1986) and Holst and Edwanger (1982). Laboratory culture: Obtained from Geobotanischen Institute, Zurich, Switzerland. Cultivation method: Cultures were grown in revised Hoaglands medium with pH 4.6 to 5.4; medium was renewed weekly. Acclimation period was 8 weeks. Plants were not removed from medium prior to measurement; Plant density not given. Controls consisted of lemna cultures without ethanol in each experiment.

Dilution water source not specified.

Growth/test medium chemistry: Hoaglands. Water hardness 636 mgll as CaCO3; Alkalinity 23 mg/l as CaCO3, Conductivity 5000 micromhos/cm, pH 4.5 to 5.1.

Exposure vessel type: 250 ml vessels; Shimadzu closures covered with paraffin. Each concentration replicated 3 times

Water chemistry (pH) on test: pH ranged 4.6 to 5.1..

Stock solution preparation: Not described.

Light levels and quality during exposure: Mean lux 5382 +/89 during exposure.

Test design: Ethanol was tested three times at each concentration (1.0 to 21 ,000 mgll, plus control). Only nominal concentrations were used.

Method of calculating mean measured concentrations: Only nominal concentrations were used.

Statistical method: EC50 - regression analysis; NOEL: Dunnett's test.
Test highly reliable.

Cells removed before measurement: Unclear. Plant fronds counted visually. Biomass measured by dry weight of plants and fronds

Biological observations:
+Cell density at each flask/each measuring point: Not applicable.
+Growth curves: Not shown.

Percent biomass/growth rate inhibition per concentration
Observations: Results were not given for each of the 21 occurrences. %

Result

The EC50 (4690 mg/l) was within the 95% confidence interval 81 to 167.764 mg/l for plant growth. The EC50 for biomass (dry weight) was 6986 mg/l (3155 to 10,817) mg/l. Of three other clones of lemna minor, 7120 and 7136 were much more resistant to ethanol with EC50 values of at least 10,000 mg/l and NOEL values of at least 1000 mg/l.

Conclusion

Ethanol was the least toxic of 8 compounds tested.

Reliability	(1) valid without restriction
Reference	Cowgill, U., Milazzo, D., Landenberger. B. (1991). The senisitivity of lemna gibba G-3 and four clones of lemna minor to eight common chemicals using a 7-day test, Res. J. Water Pollut. Control Fed. 63: 991-998.
11.11.2004	(110)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Selenastrum capricornutum (Algae)
Endpoint	growth rate
Exposure period	4 day(s)
Unit	mg/l
NOEC	< 500 measured/nominal
LOEC	= 500 measured/nominal
EC50	= 10000 measured/nominal
Limit test	
Analytical monitoring	No
Method	other
Year	1996
GLP	no data
Test substance	ethanol (64-17-5)
Method	Growth rate measured as chlorophyll content and biomass accumulation at concentrations of 0.05% (500 mg/l) and higher (range 500 to 10,000 mg/l).
Remark	Cells removed before measurement: cells were not removed. Biological observations: +Cell density at each flask/each measuring point: Not given. +Growth curves: Chlorophyll content plotted over time for each concentration, including control. Percent biomass/growth rate inhibition per concentration Observations at 500, 1000, 2000,5000 and 10,000 mg/I, the growth inhibition was 14%, 19%,26%,37% and 48% EPA guidance from 1975 recommends maximum solvent concentration of 0.05% and 0.01% for acute and chronic tests and higher concentrations often occur in practice. Ethanol as solvent in such tests has a significant effect on growth rate of the test alga. Laboratory culture: Obtained from EPA at Corville, OR. Cultivation method: Cultures were grown in Algal Assay Procedure (1971) medium in 500 ml flasks containing 250 ml algal suspension.

	Cells were not removed from medium prior to measurement; Gell density not given. Controls consisted of algal suspensions without solvent in each experiment. Dilution water source not specified. Growth/test medium: Algal Assay Procedure (1971) medium with 15 mg/I NaHC03 and 12 mg/I K2HP04. Exposure vessel type: 20 x 125 mm test tubes containing about 20 ml of suspension and ethanol. 3 Tubes per test concentration were used. Water chemistry (pH) on test: Not described. Stock solution preparation: Not described. Light levels and quality during exposure: 100 microElml\2-sec except when reduced to 1.5 microElml\2-sec 20 min before and during measurement of chlorophyll content by fluorescence. Test design: Ethanol was tested three times at each concentration (0%, 0.05%, 0.1%, 0.2%, 0.5% and 1%). Method of calculating mean measured concentrations: Only nominal concentrations were used.
Result	Growth was inhibited 48% at an ethanol concentration of 10,000 mg/I, the value approximating the EC50. Growth inhibition was 14% at 500 mg/1. Growth was significantly (p=0.05) inhibited at all concentrations of ethanol.
Reliability	(1) valid without restriction
Reference	El Jay, A. (1996) Toxic effects of organic solvents on the growth of Chiarella vulgaris and Selenastrum capricornutum. Bull. Environ. Contam. Toxicol. 57: 191-198.
11.11.2004	(109)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Chlamydomonas sp. (Algae)
Endpoint	growth rate

Exposure period	2 day(s)
Unit	g/l
NOEC	= 7.89 measured/nominal
LOEC	= 19.7 measured/nominal
EC50	
Limit test	
Analytical monitoring	no data
Method	other
Year	1980
GLP	no data
Test substance	ethanol (64-17-5)

Method

Ethanol concentrations were 0.5, 1.0, 2.5 and 5.0 %v/v (equivalent to 3.95, 7.89,19.7 and 39.5gl1 respectively) in stocks grown on agar slants at 25 degC with continuous aeration and diurnal light cycle of 12 hr. Before counting, 5% glutaraldehyde added to test systems.

Species: Chlamydomonas eugametos.

Remark

Note whether cell removed prior to measurement: 5% glutaraldehyde was added to test systems. 1 ml samples analyzed by haemocytometer or Coulter counter.

Biological observations: #Cell density: Absolute measurements not given Growth curves: Not given %Biomass/growth rate inhibition: No inhibition at ethanol concentrations of 0.5 or 1.0%/ At 2.5% cell number was 57% of control. At 5.0%, growth was completely inhibited Observations: None described.
Test organism: Bacteria-free Chiamydomonas eugametos culture collection NO.9.
Method of cultivation: Stocks grown on agar slants, liquid cultures made 3-4 days before assay Liquid cultures grown at 25 degC with continuous aeration and diurnal light cycle of 12hr.
Controls were used but are not dicussed. Tests for ethanol and other solvents were controls for tests for herbicides dissolved in these solvents.
Test conditions: temperature 25 degC.
Growth/Test medium chemistry: Not described. Grown in nutrient medium.
Dilution water source: Not described.
Exposure vessel type: 150 ml in 250 Erlenmeyer flasks aerated. 1x10"6 cells suspended in 20ml nutrient medium in 50 ml flasks not aerated.
Water chemistry in test (pH):Not described.
Stock solutions preparation: Not described.

	Light levels and quality: 12 h diurnal at 200 microEm"2/s PPFD. Test design: Solvents including ethanol were tersted at 4 concentrations, each concentration was tested at least twice. Method of calculating mean measured concentrations: Not described, Statistical test: Duncan's Multiple Range.
Result	Cell number was 57% of control at 2.5% (19.7g/l) and there was complete inhibition at 5% (39.5g/I).
Reliability	(2) valid with restrictions
Reference	Hess, F. (1980). A Chlamydomonas algal bioassay for detecting growth inhibitor herbicides. Weed Sci. 28(5}:515-520.
11.11.2004	(111)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Skeletonema costatum (Algae)
Endpoint	
Exposure period	5 day(s)
Unit	mg/l
NOEC	= 3240 - 5400
EC50	= 10943 11619
Limit test	
Analytical monitoring	no data
Method	other
Year	1989
GLP	no data
Test substance	other TS: 100% dehydrated ethanol (64-17-5)
Method	Growth inhibition in Skeletonema costatum evaluated by cell number count.
Remark	Laboratory culture: Bigelow Lab. for Ocean Sciences, West Boothbay Harbour, Maine, USA. Cultured in revised ASP12 medium at 20degC with 14 hr light at 4304 lux +1- 161/day. Agitated daily and transferred every 7 days. Acclimated for 4 weeks. Test temperature 19.5 to 20.6 degC. Controls consisting of Skeletonema in medium without ethanol were used. Temperature range 19.5-20.6 deg C. GrowthfTest medium chemistry: Not described. Dilution water source: Not described. Exposure vessel type: 100 ml covered with parafilm; each concentration tested in triplicate. Stock solutions prepared with double-distilled sterile water.

	Light levels and quality: Mean lux 4304 +/- 8.2 with a 14 h light/10 h dark cycle. Test design: 5 or more concentrations plus control each replicated 3 times. Method of calculating mean measured concentrations: Only nominal concentrations used. Statistical methods: Not described. Note whether cells removed prior to measurement: Not stated. Biological observations: #Cell density at each flask at each measuring point: Not given. #Growth curves: Not given but growth was stimulated before inhibition began. Percent biomass/growth rate inhibition, observations: Not given.
Result	EC50 for total cell count was 11,619 mg/L (7923 to 15,314) and for total cell volume, 10943 mg/L (7061 to 14,826) mg/L.
Conclusion	The authors state that, using EPA criteria, ethanol can be judged 'practically nontoxic, by this test. Ethanol was used as a carbon source, stimulating growth before inhibition began.
Reliability	(2) valid with restrictions
Reference	Cowgill, U.M., Milazzo, D.P., Landenberger, B.D. Toxicity of nine benchmark chemicals to Skeletonema costatum, a marine diatom. Environ Toxicol Chem 1989;8(5): 451-455.
11.11.2004	(112)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Chiarella pyrenoidosa (Algae)
Endpoint	growth rate
Exposure period	10 day(s)
Unit	mg/l
EC50	= 1180
Limit test	
Analytical monitoring	no data
Method	other
Year	1988
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Alga: Chiarella pyrenoidosa from National Research Council of Canada. Culture: Axenic in 250 Erlenmeyer f1asks containing nitrogen

	free medium incubated at 25 degC End point: Growth (biomass) measured by optical density over time. Concentration of ethanol: 0.4 to 3.0% Exposure period: 10 to 14 days (precise duration not specified). EC50 value was the concentration required to cause a 50% reduction in growth. Result was converted from an EC50 value of 1.18% v/v. Stratton also studied the effects of ethanol on 5 further species of algae, using the same system but with the concentration of ethanol tested ranging from 0.1 to 8%. The reported EC50 values were as follows: Anabaena sp. 6312 mg/l A. variabilis 10020 mg/l A. inaequalis 8048 mg/l A. cylindrica 7653 mg/l Nostoc sp. 22644 mg/l Test sustance was absolute ethanol.
Reliability	(2) valid with restrictions
Reference	Stratton, GW. & Smith, T.M. (1988) Interaction of organic solvents with the green alga Chlorella pyrenoidosa. Bull. Environ. Contam. Toxicol. 40:736-742. Stratton, G.W. (1987) Toxic effects of organic solvents on the growth of blue-green algae. Bull. Environ. Contam. Toxicol. 38:1012-1019
11.11.2004	(113) (114)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Cyclotella sp. (Algae)
Endpoint	Biomass
Exposure period	4 day(s)
Unit	g/l
EC50	> 2.37 measured/nominal
Limit test	
Analytical monitoring	no data
Method	other
Year	1995
GLP	no data
Test substance	ethanol (64-17-5)
Method	Species of marine diatom from the intertidal region of the Gulf of Mexico were maintained and tested in Guillard's f/2 medium enriched with artificial sea salt mix.

	A 1 % (v/v) solution of ethanol was further diluted with test medium at concentrations of 0.2,0.25 and 0.3 ml/100ml (1.58, 1.97, 2.37g/1 respectively). Tests were carried out in test tubes containing 25 ml medium and in triplicate. Each tube was inoculated from exponentially growth cells at an initial density of 4000 cells/ml. The culture was incubated on a shaker for 96 hat 30 degC under cool white light producing 100 muEm-2s irradiation in continuous cycle. Growth was measured spectrophotometrically at 525nm. Statistical analysis was by Student's ttest with significance at p<0.05.
Result	There was no significant effect on the growth rate.
Reliability	(4) not assignable Only a very limited range of concentrations was studied which in most cases produced no effect on growth. No chemical monitoring was carried on the solutions prepared. Results are only reported in summarized, basic, graphical form and only as a percentage of control response. There are insufficient data reported.
Reference	Tadros, M.G., Phillips, J., Patel, H., Pandiripally, V. Differential response of marine diatoms to solvents. Bull Environ Contam Toxicol 1995, 54 (6): 924-929.
11.11.2004	(115)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Navicula sp. (Algae)
Endpoint	Biomass
Exposure period	4 day(s)
Unit	g/l
EC50	> 2.37 measured/nominal
Limit test	
Analytical monitoring	no data
Method	other
Year	1995
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Species of marine diatom (Navicula saprophila species) from the intertidal region of the Gulf of Mexico were maintained and tested in Guillard's f/2 medium enriched with artificial sea salt mix. A 1% (v/v) solution of ethanol was further diluted with test medium at concentrations of 0.2,0.25 and 0.3 ml/l100ml (1.58, 1.97, 2.37 g/1 respectively). Tests were carried out in test tubes containing 25 ml medium and in triplicate. Each tube was

	inoculated from exponentially growth cells at an initial density of 4000 cells/ml. The culture was incubated on a shaker for 96 h at 30 deg C under cool white light producing 100 muEm-2s irradiation in continuous cycle. Growth was measured spectrophotometrically at 525nm. Statistical analysis was by Student's ttest with significance at p<0.05.
Result	There was an apparent increase in growth rate but no clear dose response relationship.
Reliability	(4) not assignable Only a very limited range of concentrations was studied which in most cases produced no effect on growth. No chemical monitoring was carried on the solutions prepared. Results are only reported in summarized, basic, graphical form and only as a percentage of control response. There are insufficient data reported.
Reference	Tadros, M.G., Phillips, J., Patel, H., Pandiripally, V. Differential response of marine diatoms to solvents. Bull Environ Contam Toxicol 1995, 54(6): 924-929.
11.11.2004	(115)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Nitzschia sp. (Algae)
Endpoint	Biomass
Exposure period	4 day(s)
Unit	g/l
EC50	
Limit test	
Analytical monitoring	no data
Method	other
Year	1995
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Species of marine diatom (Nitzschia dissipata species) from the intertidal region of the Gulf of Mexico were maintained and tested in Guillard's f/2 medium enriched with artificial sea salt mix. A 1% (v/v) solution of ethanol was further diluted with test medium at concentrations of 0.2, 0.25 and 0.3 ml/100ml (1.58, 1.97, 2.37gl1 respectively). Tests were carried out in test tubes containing 25 ml medium and in triplicate. Each tube was inoculated from exponentially growth cells at an initial density of 4000 cells/ml. The culture was incubated on a shaker for 96 h at 30 degC under cool white light producing 100 muEm-2s irradiation in continuous cycle. Growth was measured

	spectrophotometrically at 525nm. Statistical analysis was by Student's ttest with significance at p<0.05.
Result	There was a dose reponse decrease in growth but with promotion at the lower concentration, the decrease in growth at the higher concentration was only limited. The results is therefore difficult to interpret.
Reliability	(4) not assignable Only a very limited range of concentrations was studied which in most cases produced no effect on growth. No chemical monitoring was carried on the solutions prepared. Results are only reported in summarized, basic, graphical form and only as a percentage of control response. There are insufficient data reported.
Reference	Tadros, M.G., Phillips, J., Patel, H., Pandiripally, V. Differential response of marine diatoms to solvents. Bull Environ Contam Toxicol 1995, 54 (6): 924-929.
11.11.2004	(115)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	other algae: Cylindricotheca sp.
Endpoint	Biomass
Exposure period	4 day(s)
Unit	g/l
IC50	= 1.97 measured/nominal
Limit test	
Analytical monitoring	no data
Method	other
Year	1995
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Species of marine diatom from the intertidal region of the Gulf of Mexico were maintained and tested in Guillard's f/2 medium enriched with artificial sea salt mix. A 1 % (v/v) solution of ethanol was further diluted with test medium at concentrations of 0.2, 0.25 and 0.3 ml/100ml (1.58,1.97, 2.37g/l respectively). Tests were carried out in test tubes containing 25 ml medium and in triplicate. Each tube was inoculated from exponentially growth cells at an initial density of 4000 cells/ml. The culture was incubated on a shaker for 96 h at 30 deg C under cool white light producing 100 muEm-2s irradiation in continuous cycle. Growth was measured spectrophotometrically at 525nm. Statistical analysis was by Student's ttest with significance at p<0.05.

Result	There was a significant dose response decrease with an apparent IC50 of around 0.25m1/100ml (equivalent to 1.97g/l). However, taking all results from the study into account, the authors describe ethanol to be non-toxic.
Reliability	(4) not assignable Only a very limited range of concentrations was studied which in most cases produced no effect on growth. No chemical monitoring was carried on the solutions prepared. Results are only reported in summarized, basic, graphical form and only as a percentage of control response. There are insufficient data reported.
Reference	Tadros, M.G., Phillips, J., Patel, H., Pandiripally, V. Differential response of marine diatoms to solvents. Bull Environ Contam Toxicol 1995, 54 (6): 924-929.
11.11.2004	(115)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	other algae: Thalassiosira weissflgii sp.
Endpoint	Biomass
Exposure period	4 day(s)
Unit	g/l
EC0	> 2.37 measured/nominal
Limit test	
Analytical monitoring	no data
Method	other
Year	1995
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)

Method

Species of marine diatom from the intertidal region of the Gulf of Mexico were maintained and tested in Guillard's f/2 medium enriched with artificial sea salt mix.

A 1 % (v/v) solution of ethanol was further diluted with test medium at concentrations of 0.2,0.25 and 0.3 ml/100ml (1.58. 1.97. 2.37g/1 respectively). Tests were carried out in test tubes containing 25 ml medium and in triplicate. Each tube was inoculated from exponentially growth cells at an initial density of 4000 cells/ml. The culture was incubated on a shaker for 96 h at 30 degG under cool white light producing 100 muEmM2s irradiation in continuous cycle. Growth was measured spectrophotometrically at 525nm. Statistical analysis was by Student's ttest with significance at $p<0.05$.

Result There was an apparent increase in growth rate but no clear dose response relationship.

Reliability	(4) not assignable Only a very limited range of concentrations was studied which in most cases produced no effect on growth. No chemical monitoring was carried on the solutions prepared. Results are only reported in summarized, basic, graphical form and only as a percentage of control response. There are insufficient data reported.
Reference	Tadros, M.G., Phillips, J., Patel, H., Pandiripally, V. Differential response of marine diatoms to solvents. Bull Environ Contam Toxicol 1995, 54 (6): 924-929.
11.11.2004	(115)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Scenedesmus subspicatus (Algae)
Endpoint	growth rate
Exposure period	
Unit	mg/l
IC10	= 400 measured/nominal
Limit test	
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Reliability	(4) not assignable
Reference	Schmidt C et al (1988) Structure activity relationship of organic substances and bioindicators. Vom Wasser, 70, 21-32.
11.11.2004	(116)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Scenedesmus subspicatus (Algae)
Endpoint	other: inhibition of protoplast O2 production
Exposure period	
Unit	mg/l
IC10	= 460 measured/nominal
Limit test	
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Reliability	(4) not assignable
Reference	Schmidt C et al (1988) Structure activity relationship of organic

	substances and bioindicators. Vom Wasser, 70, 21-32.
11.11.2004	(116)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Chlorococcum sp. (Algae)
Endpoint	Biomass
Exposure period	24 hour(s)
Unit	mg/l
EC50	> 1000
LC100	
Limit test	
Analytical monitoring	no data
Method	other
Year	
GLP	
Test substance	95 – 99.9% ethanol (64-17-5)
Method	In fresh water; method not specified.
Reliability	(4) not assignable
Reference	Krebs, F. (1991) Deutsche Gewasserkundliche Mitteilungen 35 (5/6):161-170.
29.09.2003	(117)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Dunaliella bioculata (Algae)
Endpoint	Biomass
Exposure period	2 day(s)
Unit	mg/l
EC50	= 1000 measured/nominal
LC100	=.05
Limit test	
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Two concentrations of ethanol were tested, 0.1% (1000 mg/I) and 0.05% (500 mg/l).
Result	Growth was reduced 10% at 1000 mg/1. The NOEC and LOEC were not calculated.
Reliability	(4) not assignable
Reference	Felix, H.R., Challel, R., Harr, J. Use of the cell wall-less alga Dunaliella bioculata in herbicide screening tests. Ann Appl Biol

	1988; 113 (1): 55-60.
11.11.2004	(118)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Microcystis aeruginosa (Algae, blue, cyanobacteria)
Endpoint	Biomass
Exposure period	8 day(s)
Unit	mg/l
EC0	= 1450 measured/nominal
Limit test	
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Difference in growth rate between ethanol-containing cultures and controls measured turbidimetrically. Toxic threshold concentration determined.
Reliability	(4) not assignable
Reference	Bringmann, G. & Kuhn, R. (1976) Vergleichende Befunde der Schadwirkung wassergefaehrdender Stoffe gegen Bakterien (Pseudomonas putida) und Blaualgen (Microcystis aeruginosa). gwf-wasser/abwasser 117, 410 - 413.
11.11.2004	(119)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Scenedesmus quadricauda (Algae)
Endpoint	growth rate
Exposure period	7 day(s)
Unit	mg/l
LOEC	= 5000
Limit test	
Analytical monitoring	No
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Ethanol tested in double-distilled water in a cell multiplication inhibition test. Endpoint measured was the toxic threshold.
Reliability	(4) not assignable
Reference	Bringmann, G. & Kuhn, R. (1980) Comparison of the toxicity

	thresholds of water pollutants to bacteria, algae, and protozoa in the cell multiplication inhibition test. Water Res. 14, 231 to 241.
11.11.2004	(120)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Preferred Value	
Test Substance:	n-Butyl Alcohol
Method:	OECD 201, USEPA TSCA 40 CFR 797.1050
Year (guideline):	1984,1994
Type (test type):	Static Algal Toxicity Test
GLP:	Yes
Year (study performed):	1998
Species:	Freshwater green alga (Selenastrum capricornutum)
Analytical Monitoring:	Yes
Exposure Period:	96 Hours
Statistical Method:	(FT -ME)*Linear interpolation for EC values, Dunnett's test for NOAEC
Test Conditions:	(FT - TC)Test solutions were prepared by diluting a 50-mg/mL stock solution of n-butyl alcohol (99.9% purity) with laboratory-prepared algal nutrient medium to nominal concentrations of 125, 250, 500, 1000, and 2000 mg/L. Stock solution was also prepared with nutrient medium. Test vessels were sterile, 250-mL Erlenmeyer flasks plugged with foam stoppers and contained 100 mL.of test or control (nutrient medium) solution. Vessels were continuously shaken mechanically at 100 rpm. Three replicate vessels were maintained for each treatment and control group. Initial cell density was 1.0 x 10 4 cells/mL (nominal). Samples were collected from each replicate test vessel at each 24-hour interval and held at 4°C until cell density measurement. Cell counts were obtained using an electronic particle counter (Coulter Electronics, Inc.). Cell densities were used to calculate growth inhibition values and effects concentrations (ECIO, EC50, and EC90) relative to the control. Algal growth inhibition was differentiated as algicidal or algi static effects at test termination by subculturing test solutions with maximally inhibited growth to fresh nutrient medium for a 9-day recovery period. Water samples for analytical verification were collected at test initiation from the preparation vessels of each treatment and the controL Samples collected at test termination were a composite of the replicates for each treatment and the control and were filtered to remove the algae prior to analysis. Temperature ranged from 23.2 to 25.3 cC. Light was continuous

at 4240 to 4568 lux. Measurements of pH 7.4 at test initiation and ranged from 6.8 to 7.7 at 96 hours.

Original algal cultures were obtained from UTEX The Culture Collection of Algae at the University of Texas at Austin and were maintained in culture medium for at least two weeks prior to testing.

Based on Day 0 measured n-butyl alcohol concentrations:
96-hour ECl0 = 134 mg/L (95% CL: 124 - 167 mg/L)
96-hour EC50 = 225 mg/L (95% CL: 204 - 246 mg/L)
96-hour EC90 = 717 mg/L (95% CL: 586 - 809 mg/L)

96-hour growth rate inhibition:

Day 0 Measured Concentration (mg/L)	96-hour % Inhibition	96-hour Cell Density
Control	--	4,206,362
129	7.7	3,883,813
241	57	1,808,913*
491	83	732,225*
1010	100	15,521*
1980	100	15,754*

* Indicates significant difference from control using Dunnett's test (p <= 0.05)

Changes in cell density indicated that exponential growth occurred in the control replicates. The coefficient of variation for the control replicates was 8.5%.

Algal cells in 1980 mg/L (2000mg/L nominal) resumed normal growth after 9 days. Effects on algal growth were considered algi static.

Measured concentrations of test solutions at test initiation ranged from 97 to 103% of nominal values. Measured concentrations after 96 hours ranged from <LOQ to 73% of nominal.

n-Butyl Alcohol concentrations in test chambers were determined using a Hewlett-Packard Model 5890 Gas Chromatograph with flame ionization detector.

Reliability: (1) Reliable without restriction.

	OECD endpoints were not determined.
Reference:	Wong, D.C.L, P.B. Dorn, and J.P. Salanitro. 1998. Aquatic Toxicity of Four Oxy-Solvents. Equilon Enterprises, LLC Technical Information Record WTC-3520.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance:	1-Butanol
Test species:	Scenedesmus subspicatus (Green Algae)
Test method:	DIN Test Method 38412 Part 9
GLP:	No
Test results:	96 Hr. EC10 >500 mg/l 96 Hr. EC50 >500 mg/l 96 Hr. EC90 >500 mg/l
Reliability:	(2) valid with restrictions, full experimental data not presented
Reference:	BASF Corp. Internal Report dated 9/19/91.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance:	1-butanol (71-36-3)
Value:	361 mg/L
Remark:	An acute 96-h EC50 for green algae was calculated using ECOSAR, from the USEP A. The preferred physical properties were used. The SAR for esters was employed. The structure was determined from the CAS RN as stored in the accompanying database of SMILES notations within ECOSAR. Chemical-specific input parameters were: molecular weight (74.12 g/mol), vapor pressure (0.56 hPa or 0.42 mm Hg), log Kow (0.88), melting point -89.9° C, aqueous solubility 77,000 mg/L, boiling point of 117.6° C, and a Henry's Law constant of 5.3 E- 7 atm-m3/mol.
Reliability:	(2) valid with restriction, calculated value
Reference:	EPA's ECOSAR model (v. 0.991). EPISUITE v.3.l0, U.S. Environmental Protection Agency, April (2001).

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: Selenastrum capricornutum (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l
Analytical monitoring: yes
NOEC: = 11.3
LOEC: = 31.2

EC10: = 19.8
EC50: = 79.7
Limit Test: no

Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 2005
GLP: yes
Test substance: >95% 1-hexanol (111-27-3)

Method: Test condition:

TEST ORGANISMS
Strain: Pseudokirchneriella subcapitata
Source/Supplier: SAG, Culture Collection of Algae at Pflanzenphysiologisches Institut of the University at Göttingen, Albrecht von Haller Institut, Untere Klarspüle 2, D-37073 Göttingen, Catalog No 61.81.

Pretreatment: The stock cultures were maintained fulfill the criteria of the OECD guidelines. Prior to testing a pre-culture was established in test medium to obtain exponentially growing algae for the test.

STOCK AND TEST SOLUTION AND THEIR PREPARATION
A stock solution was prepared by adding 180 mg of the test substance to sterilized test medium and adjusting the volume to 1 L. The solution was stirred for 24 hours. The highest test concentration was diluted with sterilized growth medium to obtain the other four nominal test concentrations under sterile conditions: 7.7, 17, 37, 82 and 180 mg hexanol/L.

ANALYSIS OF EXPOSURE CONCENTRATIONS
Samples of fresh and old test media, with and without algae present were analysed to determine the concentration of the test substance. The analyte was extracted from the algae test samples by liquid-liquid partitioning with n-hexane. After shaking and settling the n-hexane extract was removed and the analyte derivatized using MSTFA. Measurement was performed by GC-MS in SIM mode using internal standard calibration with deuterated n-hexanol as internal standard.

STABILITY OF TEST CHEMICAL SOLUTIONS
The mean measured test concentrations varied in some cases by more than +/-20% of the nominal values. The results are therefore interpreted with respect to the mean measured values.

DILUTION WATER
Source: A sterilized synthetic growth medium according to OECD 201
Aeration: None reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported

TEST SYSTEM
Concentrations: 7.7, 17, 37, 82 and 180 mg hexanol/L (nominal), 4.72, 11.3, 31.2, 50.1 and 111.2 mg/L (mean measured with algae present), 5.48, 12.3, 29.3, 54.9 and 105.5 mg/L (mean measured without algae present)
Renewal of test solution: None
Exposure vessel type: Test vessels are 250 mL conical glass flasks covered with silicone-sponge caps. The vessels and caps were sterilized prior to use (autoclaving or heating). The cultures were resuspended continuously by shaking on a laboratory shaker (Incubation Shaker Multitron ®, INFORS, Switzerland).
Number of replicates: Controls: Six replicate control cultures containing only culture medium and algal suspension under sterile conditions. Three replicates of each test concentration.
Initial cell concentration: 10,000 cells/mL.
Test temperature: 22.0 - 22.2 °C
Dissolved oxygen: Not reported
pH: 8.52 - 8.58 (Controls), 8.08 - 8.40 (testconcentrations)
Intensity of irradiation: 8000 Lux
Photoperiod: Exposed to constant lighting.

TEST PARAMETER:
End point: Growth measured as changes in cell number that were subsequently analysed with respect to growth rate and biomass.
Method of measurement: Cell concentrations were determined using an electronic particle counter (CASY 1 Model TT, Schärfe System, Reutlingen, Germany). The correctness of the electronic counts was checked by microscopically counting following internal standard operation procedures

Result: Based on mean measured exposure concentrations
EbC10: = 4.97
EbC50: = 20.5
LOEC: = <4.72
NOEC: = <4.72

Reliability: (1) valid without restriction

Flag: Critical study for SIDS endpoint

Reference: Wenzel, A. (2005). Alga, Growth Inhibition Test. Effect of hexanol on the growth of the green alga Pseudokirchneriella subcapitata. Fraunhofer-Institute for Molecular Biology and Applied Ecology (IME), Schmallenberg, Germany. GLP Code: SDA-003/4-30.

21-DEC-2005 (81)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: Scenedesmus quadricauda (Algae)
Endpoint: biomass
Exposure period: 8 day(s)
Unit: mg/l
Analytical monitoring: no data
TT : = 30
Limit Test: no

Method: other
Year: 1978
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability scores) but with higher toxicity values are available.

Reference: Bringmann, G. and Kuhn, R. 1978. Testing of substances of their toxicity threshold: Model organisms Microcystis (Diplocystis) aeruginosa and Scenedesmus quadricauda. Mitt. Internat. verein. Limnol. 21: 275-284.

Bringmann, G. and Kuhn, R. 1980. Comparison of the toxicity thresholds of water pollutants to bacteria, algae, and protozoa in the cell multiplication inhibition test. Water Research 14: 231-241.

29-DEC-2005 (12) (14)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: Euglena sp. (Algae)
Endpoint: growth rate
Exposure period: 7 day(s)
Unit: mg/l
Analytical monitoring:
LOEC: = 75

Method: other: not specified

Year: 1980
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
Reference: Bringham, G. and Kuhn, G. Comparison of the Toxicity Threshold of Water Pollutants to Bacteria, Algae, and Protozoa in the Cell Multiplication Inhibition Test. Water Res., Vol. 14, No. 3, pgs. 231-241, 1980.
20-OCT-2005 (11)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: Scenedesmus quadricauda (Algae)
Endpoint: growth rate
Exposure period: 7 day(s)
Unit: mg/l
Analytical monitoring: no
LOEC: = 30
Test substance: >95% 1-hexanol (111-27-3)
Method: other: not specified
Year: 1980
GLP: no data

Remark: This is the concentration in which a 3% in extinction value occurred.
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
Reference: Bringham, G. and Kuhn, G. Comparison of the Toxicity Threshold of Water Pollutants to Bacteria, Algae, and Protozoa in the Cell Multiplication Inhibition Test. Water Res., Vol. 14, No. 3, pgs. 231-241, 1980.

Bringmann, G. and Kuhn, R. 1980. Comparison of the toxicity thresholds of water pollutants to bacteria, algae, and protozoa in the cell multiplication inhibition test. Water Research 14: 231-241.
20-OCT-2005 (11) (14)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: other algae: Chilomonas paramecium
Endpoint: growth rate
Exposure period: 48 hour(s)
Unit: mg/l
Analytical monitoring: no
LOEC: = 18
Test substance: >95% 1-hexanol (111-27-3)
Method: other: not specified
Year: 1980
GLP: no data

Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
Reference: Bringham, G. and Kuhn, G. Comparison of the Toxicity Threshold of Water Pollutants to Bacteria, Algae, and Protozoa in the Cell Multiplication Inhibition Test. Water Res., Vol. 14, No. 3, pgs. 231-241, 1980.
20-OCT-2005 (11)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: other algae: Enteromorpha intestinalis
Endpoint: other: ion retention
Exposure period: 2 minute(s)
Unit: mg/l
Analytical monitoring: no data
EC50: = 400

Method: other
Year: 1980
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Method: Samples of E. intestinalis comprising several pieces of thallus from different specimens (total weight 1 g) were risnsed once in distilled water for 3 seconds then placed in 50 ml of distilled water in a beaker and left for 2 min (sample 1). The E. intestinalis was then transferred to lidded bottles containing a further 50 ml of distilled water then placed in a boiling water bath. After 5 min the bottles were

removed from the bath and the contents poured through a plastic sieve into a 100 ml beaker (sample 2). The alga was discarded. The conductivity of samples 1 and 2 was measured and used to derive an ion retention health index. This index reflects the proportion of the total leechable ions present in the thallus which were retained after exposure to distilled water for 2 mins. The index was calculated by dividing the conductivity of sample 2 by the total conductivity (i.e. sample 1 + sample 2).

Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability scores) but with lower effect values are available.

Reference: Schild, R., Donkin, P., Donkin, M.E. and Price D.N. A QSAR for measuring sublethal responses in the marine macroalga Enteromorpha intestinalis. SAR and QSAR in Environmental Research, 4(2-3), 147-154.

20-OCT-2005 (57)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Species: Scenedesmus subspicatus (Algae)
Endpoint: other: growth rate and biomass
Exposure period: 48 hour(s)
Unit: mg/l
Analytical monitoring: no data
EC10: = 2.8 - 4.2
EC50: = 6.5 - 14
Limit Test: no

Method: other
Year: 1989
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Method: Modified Test Procedure incorporating DIN 38 412, Part 9 and account also being taken of the Test Methods using Water Organisms, DIN 38 412, Part 1.

Result: RESULTS: EXPOSED
Biomass EbC50 = 6.5 mg/l
Growth rate ErC50 = 14 mg/l
Based on nominal concentrations

Reliability: (4) not assignable
Documentation insufficient for assessment.

Flag: Critical study for SIDS endpoint

Reference: Kuhn, R. and Pattard, M. 1990. Results of the harmful effects of water pollutants to green algae (Scenedesmus

subspicatus) in the cell multiplication inhibition test.
Wat. Res. 24(1):31-38.
21-DEC-2005 (74)

1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)

Species: other algae: Enteromorpha intestinalis
Endpoint: other: ion retention
Exposure period: 2 minute(s)
Unit: mg/l
Analytical monitoring: no data
EC50: = 120
Limit Test: no

Method: other
Year: 1980
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Method: Samples of E. intestinalis comprising several pieces of thallus from different specimens (total weight 1 g) were risnsed once in distilled water for 3 seconds then placed in 50 ml of distilled water in a beaker and left for 2 min (sample 1). The E. intestinalis was then transferred to lidded bottles containing a further 50 ml of distilled water then placed in a boiling water bath. After 5 min the bottles were removed from the bath and the contents poured through a plastic sieve into a 100 ml beaker (sample 2). The alga was discarded. The conductivity of samples 1 and 2 was measured and used to derive an ion retention health index. This index reflects the proportion of the total leechable ions present in the thallus which were retained after exposure to distilled water for 2 mins. The index was calculated by dividing the conductivity of sample 2 by the total conductivity (i.e.sample 1 + sample 2).
Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability scores) but with lower effect concentrations are available.
Reference: Schild, R., Donkin, P., Donkin, M.E. and Price D.N. A QSAR for measuring sublethal responses in the marine macroalga Enteromorpha intestinalis. SAR and QSAR in Environmental Research, 4(2-3), 147-154
21-OCT-2005 (98)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Unit: mg/l

Analytical monitoring:
EC10: calculated
EC50: ca. 1 - 10

Method: other: read-across/expert judgement
Year: 2005
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Method: The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by modelling.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
Reliability: (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
Flag: Critical study for SIDS endpoint
Reference: Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (6)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)</u>

Species: Scenedesmus subspicatus (Algae)
Endpoint: other: biomass and growth rate
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EbC0 : = .4
EbC50 : = .62
ErC50 : = 2.6
Limit Test: no

Method: other: DIN 38412, Part 9 (Conforms with OECD-Guideline 201.).
GLP: yes

Test substance: other TS: Dodecanol (112-53-8)

Source: Henkel KGaA 1994d.
Test condition: TEST ORGANISMS
Strain: Scenedesmus subspicatus SAG 8681
Supplier: Institute of Plant Physiology, University of Gottingen
Pretreatment: not reported
Controls: 3 flasks served as controls
Initial cell concentration: 1*10exp4 cells/ml
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Ethanol
Concentration of vehicle, solvent:
STABILITY OF TEST CHEMICAL SOLUTIONS:
REFERENCE SUBSTANCE:
TEST SYSTEM:
Test type: static test
Loading rates: 0.1, 0.2, 0.4, 0.8, 1, 2, 4 and 8 mg/l
Renewal of test solution: None
Exposure vessel type: 300 ml Erlenmeyer flasks
Number of replicates: 3
Test temperature: 21.9-22.6 C
pH mean: 7.5-8.1
Intensity of irradiation: 2000lux
Photoperiod: continuous illumination
TEST PARAMETER: biomass and growth rate
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
References: Barilyak, I.R. et al, 1991 Embyrotoxic effects of some monoohydric alcohols. Ontogenez 22(1):71-74 (Russian language paper, translation available).

Henkel KGaA. 1994d. Lorol C12-99: Algen-Zellvermehrungshemmtest. Biological Research and Product safety/Ecology: Unpublished results; Report No. R 9400362.
13-JAN-2004 (10)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)

Species: Scenedesmus subspicatus (Algae)
Endpoint: other: growth rate and biomass
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no

NOEC: = .3
EbC0 : = .3
EbC10 : = .73
EbC50 : = .97
Limit Test: no

Method: other: DIN 38412, Part 9 (Conforms with OECD-Guideline 201.).
Year: 1992

GLP: yes
Test substance: other TS: Dodecanol (112-53-8)

Remark: Reported data refers to the effects on biomass only. The data referring to the effect on growth rate, show that up to the highest test substance concentration (10 mg/l) only <=30% inhibition was observed. Therefore, no ErC50 value was calculated in this study.
Result: RESULTS: EXPOSED
Biomass
EbC10 (0-72h) = 0.79 mg/l
EbC10 (0-96h) = 0.73 mg/l
EbC50 (0-72h) = 6.02 mg/l
EbC50 (0-96h) = 0.97 mg/l
Source: Henkel KGaA 1992.
Reliability: (2) valid with restrictions
Not key study: Other studies (same reliability score) but showing greater toxicity are available
Reference: Henkel KGaA. 1992. 1-Dodecanol: Algen-Zellvermehrungshemmtest. Biological Research and Product safety/Ecology: Unpublished results; Report No. RE 920200.
13-JAN-2004 (7)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)</u>

Species: Scenedesmus subspicatus (Algae)
Endpoint: other: growth rate and biomass
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no data
EL50 : > 10
Limit Test: no

Method: other: DIN 38412 part 9.
Year: 1992
GLP: yes

Test substance: > 95% 1-Tetradecanol (112-72-1)

Method: METHOD FOLLOWED: German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the inhibitory effect of water constituents on green algae (Algae gowth-inhibition-test)(L9); DIN 38412 part 9
This method corresponds to the OECD Guideline 201.

Remark: The solubility of C14 alcohol (Tetradecanol) is about 0.15 mg/l, therefore the LC50 was not achieved at the solubility limit. The dose-response was found above the solubility, which suggests the possibility of an artefact causing it.

Result: RESULTS: EXPOSED
Nominal/measured concentrations: nominal
Effect data/Element values:
ErL0 = 1 mg/l, ErL10 = 2.9 mg/l, ErL50 = >10 mg/l
EbL0 = 0.1 mg/l, EbL10 = 0.28 mg/l, EbL50 = >10 mg/l
Cell density data: cell densities increased from 2.3-7.3*10exp4 cells/ml after 24 hours to the following densities after 96 hours: 2.4*10exp6 (0.1 mg/l), 2*10exp6 (0.6 mg/l), 1.9*10exp6 (1 mg/l), 2.1*10exp6 (3 mg/l) and 2*10exp6 (10 mg/l).
RESULTS CONTROL: cell density increased from 4.7*10exp4 after 24 hours to 2.1*10exp6 cells/ml after 96 hours.

Source: Guhl 1992d.

Test condition: TEST ORGANISMS
Strain: Scenedesmus subspicatus SAG 8681
Supplier: Institute of Plant Physiology, University of Gottingen
Laboratory culture: not reported
Method of cultivation: not reported
Pretreatment: not reported
Controls: without test substance
Initial cell concentration: 1-10exp4 cells/ml
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: none
Vehicle, solvent: none
Other procedures: a stock solution of 0.1 g/l was stirred for 72 hours, filtered and dilutions prepared from the filtrate
STABILITY OF TEST CHEMICAL SOLUTIONS: not reported
REFERENCE SUBSTANCE: none
TEST SYSTEM:
Test type: static test
Loading rates: 0.1, 0.3, 1, 3 and 10 mg/l
Renewal of test solution: None

Exposure vessel type: 300 ml Erlenmeyer flasks
Number of replicates: 3
Test temperature: 22.5-23 C
pH mean: not reported
Intensity of irradiation: 2000lux
Photoperiod: continuous illumination
TEST PARAMETER: biomass and growth rate
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Guhl Dr. 1992d. 1-Tetradecanol: Subacute/chronic toxicity: Algae. Biological Research and Product Safety/Ecology: Unpublished results; test substance registration No. 910723; Henkel KGaA; Report No. RE 920041 (with english summary report No. R9901349).

20-OCT-2005 (21)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Species: Scenedesmus subspicatus (Algae)
Endpoint: other: growth rate and biomass
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no data
EbL50 : = 676
ErL50 : > 980
Limit Test: no

Method: other: DIN 38412 part 9.
Year: 1992
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: METHOD FOLLOWED: German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the inhibitory effect of water constituents on green algae (Algae growth - inhibition-test)(L9); DIN 38412 part 9
This method corresponds to the OECD Guideline 201.

Remark: The water solubility of hexadecanol is about 0.01 mg/l, therefore the no effect level appears to be above the saturation limit. The loading rates were all markedly above the solubility, which suggests that the dose-response is artefactual.

Result: RESULTS: EXPOSED
Nominal/measured concentrations: nominal

Effect data/Element values:
ErL0 = 98 mg/l, ErL10 = 206 mg/l, ErL50 = >980 mg/l
EbL0 = 9.8 mg/l, EbL10 = 24 mg/l, ELC50 = 676 mg/l
Cell density data: cell densities increased from 3.7-4.3*10exp4 cells/ml after 24 hours to the following densities after 96 hours: 2.2*10exp6 (10 mg/l), 1.1*10exp6 (30 mg/l), 1.2*10exp6 (100 mg/l), 9*10exp5 (300 mg/l) and 9*10exp5 (1000 mg/l).
RESULTS CONTROL: cell density increased from 2.7*10exp4 after 24 hours to 2.1*10exp6 cells/ml after 96 hours.

Source: Guhl 1992c.

Test condition: TEST ORGANISMS
Strain: Scenedesmus subspicatus SAG 8681
Supplier: Institute of Plant Physiology, University of Gottingen
Laboratory culture: not reported
Method of cultivation: not reported
Pretreatment: not reported
Controls: without test substance
Initial cell concentration: 1*10exp4 cells/ml
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: none
Vehicle, solvent: None
Other procedures: test substance directly weighed into test vessels
STABILITY OF TEST CHEMICAL SOLUTIONS: not reported
REFERENCE SUBSTANCE: none
TEST SYSTEM
Test type: static test
Concentrations: 0, 10, 30, 100, 300 and 1000 mg/l
Renewal of test solution: none
Exposure vessel type: 300 ml Erlenmeyer flasks
Number of replicates: 3
Test temperature: 22 - 23 C
pH mean: not reported
Intensity of irradiation: 2000 lux
Photoperiod: continuous illumination
TEST PARAMETER: biomass and growth rate
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

Reliability: (2) valid with restrictions

Flag: Critical study for SIDS endpoint

Reference: Guhl Dr. 1992c. 1-Hexadecanol: Subacute/chronic toxicity: Algae. Biological Research and Product Safety/Ecology: Unpublished results; test substance registration No. 910721; Henkel KGaA, Report No. RE 920039 (with english summary report No. R9901354)

20-OCT-2005 (36)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Species: Scenedesmus subspicatus (Algae)
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring:
EC0: = 10
EC50: = 690

Method: other: DIN 38412, Teil 9 (Algal growth inhibition test)
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Related to: Test substance
Source: Henkel KGaA Duesseldorf
Test substance: Active Matter = 98 %.
Reliability: (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Reference: IUCLID Data Set: 1-Hexadecanol. Shell Chemicals Ltd. May 11, 2006.
11-SEP-2005

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Species: Scenedesmus subspicatus (Algae)
Endpoint: biomass
Exposure period: 96 hour(s)
Unit: mg/l
Analytical monitoring: no
EC10: = 26
EC50: = 250
Limit Test: no

Method: other: DIN 38412, Part 9
Year: 1992
GLP: yes
Test substance: other TS: Octadecanol (112-92-5)

Remark: Test method conforms with OECD-Guideline 201.
Result: RESULTS: EXPOSED
EC0 = < 10 mg/l (due to variability in cell density, the EC0 could not be reliably determined)

EC10 = 26 mg/l
EC50 = 250 mg/l
Based on nominal concentrations
The water solubility of Octadecanol is about 0.001 mg/l,
therefore the EC50 is well above the solubility limit.

Source: Guhl 1992b.

Test condition: TEST ORGANISMS
Strain: Scenedesmus subspicatus
Supplier: Institute for plant physiology, University
Gottingen
Pretreatment: not reported
Controls: 3 replicates
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: not reported
Concentration of vehicle, solvent: not reported
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: not reported
Aeration: not reported
Alkalinity: not reported
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: 10, 30, 100 and 300 mg/l (Unfiltered)
0.1, 0.3, 1.0, 3.0, 10.0 mg/l (Filtrate)
Exposure vessel type: 300 ml Erlenmeyer flasks
Number of replicates: 3
Initial cell concentration: 10000 cells/ml
Test temperature: 22-23.5 C
Dissolved oxygen: Not reported
pH mean: Not reported
Adjustment of pH: Not reported
Intensity of irradiation: 2000 Lux
Photoperiod: Constant illumination
TEST PARAMETER: biomass
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

Reliability: (2) valid with restrictions

Flag: Critical study for SIDS endpoint

Reference: Guhl, Dr. 1992b. Octadecanol (Lorol C18-98) Algenzellvermehrungshemmtest. Report Henkel KGaA Report No. RE 920040.

12-MAR-2004 (5)

<u>1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)</u>

Method: other: read across/expert judgement
Year: 2005
GLP: no
Test substance: >= 90% 1-eicosanol (629-96-9)

Method: The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by modelling.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
Flag: Critical study for SIDS endpoint
Reference: Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (5)

<u>1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)</u>

Method: other: read across/expert judgement
Year: 2005
GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Method: The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty

in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by modelling.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
Flag: Critical study for SIDS endpoint
Reference: Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (5)

1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)

Unit: mg/l
Analytical monitoring: no
LC50: = 3.82×10^{-6} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-tetracosanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99, USEPA (2006).
05-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Unit: mg/l **Analytical monitoring:** no
LC50: = 5.48×10^{-7} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-hexacosanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions

Reference: ECOSAR v0.99, USEPA (2006).
05-APR-2007

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Unit: mg/l
Analytical monitoring: no
LC50: = 7.98 x 10^{-8} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-octacosanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99, USEPA (2006).
05-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Unit: mg/l
Analytical monitoring: no
LC50: = 1.16 x 10^{-8} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-triacontanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99, USEPA (2006).
05-APR-2007

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Ceriodaphniasp. (Crustacea)
Endpoint	Mortality
Exposure period	10 day(s)
Unit	mg/l
LC50	= 1284 - 2638

Analytical monitoring	no data
Method	other
Year	1991
GLP	
Test substance	95 – 99.9% ethanol (64-17-5)

Method

Follows the basic methodology for the three brood test proposed by Mount and Norberg (Mount, D.J. and Norberg, T.J. (1984) A seven-day life cycle c1adoceran toxicity test. Environ. Toxicol. Chem. 3,425 - 434).Analytical methods used for test substance: no data given.Vehicle used: not required. Statistical methods: For LC50: Probit, moving average and nonlinear interpolation. Calculation of point estimates and other corresponding 95% confidence intervals made using a program written by Stephan (1977, Methods for calculating an LC50, In Mayer FL et al (eds), Aquatic toxicology and hazard assessment, ASTM STP 634: 65-84).
Calculation of EC50: statistical package SAS GLM (198? SAS/STAT guide for personal computers, version 6th ed, SAS institute Inc, Cary, NC) used to generate regression equations. NOELs calculated using Dunnett's t-test.Test organism: Daphnia magna strauss 1820 populations (of British origin) had been maintained in the Dow Chemical Company Laboratory since 1982 without drastic changes in population.
Population maintained at 25C for past 3 years and sustained on Ankistrodesmus convulutus {reared in medium based on Provasoli and Pintner {1968, Ecological implications of in vitro nutritional requirements of algal flagellates", Ann NY

Acad. ScL 56,839-851.) and Nitzschia frustulum Kutzing cultured in ES-I-Si, a medium developed by Provasoli (1968, "Media and prospects for the cultivation of marine algae", in Watanabe A et ai, Cultures and collections of algae, Proceedings of a US-Japan conference, Hakone 1966.) Algal diet axenic.Test conditions: The. testing conditions followed the basic tenets of the original three-brood test proposed by Mount and Norberg (1984) but were revised in that they emphasize the needs of the animals in terms of space and diet. Details of the conditions may be found in in Cowgill and Milazzo (1989).
Test vessels were wide mouth clear glass jars graduated in milliliters to contain 150mL.
Into each jar was fitted a glass tube, 3.5 cm diameter.
which had affixed to one end a nytex screen of 243 11m mesh for C. dubia or 1000 11m mesh for D. magna, These screens were affixed to the glass tubes with silicone glue. After the screens were glued to the glass tubes, three glass beads, 8 mm

in diameter, were affixed to the underside equidistant from each other. This was covered with a glass petal dish 5.5 cm in diameter. The jar containing the screened tube was filled with double distilled water and autoclaved for 10 mins at a pressure of 124 kPa. This procedure was repeated three times, renewing the distilled water each time, before the equipment was used for a test.
This procedure accomplished the complete removal of all effects of the silicone glue. Only glass vessels were used.

Remark

Species: Ceriodaphnia dubia.
Using the USEF'A classification scheme, ethanol would be classified as practically non toxic based on survival.
Based on reproductive parameters, it would be classified as slightly toxic.

Test Condition

Analysis of Lake Huron water used in culturing and testing
Al 140
NH3 total ND(l0)
B 40
Ca 18700
Cr 8
Cu 5
F 80
Fe 17
Pb (5) NO (5)
Mg 7800
Mn (5) NO (5)
K 1040
Si 3400
Na 4800
S 6000
Zn 8
Total dissolved solids 118000
Total suspended solids NA
Total organic carbon 1600

Test conditions Test vessel: Capacity 150ml, Content 100ml Screen composition: Nytex, Screen mesh size, 243j1m Ught lux: 670 ± 100 lux Photoperiod, 16 h light, 8 h dark Temperature 25 ± 2

Dissolved oxygen, 8.0 ± 1.5mg/L pH: 8.2 ± 0.2 Dilution water Hardness, as mg CaC03,1L: 90-110 Alkalinity, as mg CaCQ3/L: 55-75 Habitat: Environmental chamber Habitat changing frequency: Every other day Diet: algae (A. convolutes, N. frustulum) Feeding rate (cells/vessel): A. convolutes 9x10^6, N.

	frustulum 1.8x10^6 Feeding frequency: daily Age of organisms, <12h (all from fourth brood.) Number of control broods: 3 Permitted control loss, 20% Number of organisms/ vessel: 1 Number of organisms/Concentration: 10 Number of organismsllcontrol: 20 Test length, days: 7-10 Variables monitored Daily: light, temperature, survival, progeny Variables monitored every second day: w ater quality variables in renewed solutions Variables monitored at Test termination: Survival, total progeny, adult weight Endpoints: Survival, total progeny, dry adult weight, number of broods, mean brood size, loss of control limited to 20% (lC50/EC50/NOEC) Test ended when the control animals had produced three broods. Test concentrations used: not specified.
Reliability	(2) valid with restrictions This is a well reported study, particularly regarding the methodology of testing. The main weakness is lack of detail on test concentrations used and on the analytical method used to assess test substance concentration.
Reference	Cowgill, U.M., Milazzo, D.P. (1991) The sensitivity of Ceriodaphnia dubia and Daphnia magna to Seven Chemicals Utilizing the Three Brood Test. Arch Environ Contam Toxicol 20(2): 211-217.
11.11.2004	(125)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Ceriodaphnia sp. (Crustacea)
Endpoint	reproduction rate
Exposure period	10 day(s)
Unit	mg/l
NOEC	=9.6
EC50	26 - 38
LC50	= 1806
Analytical monitoring	no data
Method	other: see free text
Year	1984
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Follows the basic methodology for the three brood test proposed by Mount and Norberg (Mount, D.J. and Norberg, T.J. (1984) A seven-day life cycle c1adoceran toxicity test. Environ. Toxico!. Chem. 3,425 - 434).Analytical methods used for test substance: no data given.Vehicle used: not required.Statistical methods: For LC50: Probit, moving average and nonlinear interpolation. Calculation of point estimates and other corresponding 95% confidence intervals made using a

program written by Stephan (1977, Methods for calculatina an LC50. In Maver FL et al (eds). Aquatic toxicology and hazard assessment, ASTM STP 634: 65-84). Calculation of EC50: statistical package SAS GLM (1987, SAS/STAT guide for personal computers, version 6th ed, SAS institute Inc, Cary, NC) used to generate regression equations. NOELs calculated using Dunnett's t-test.Test organism: Daphnia magna strauss 1820 populations (of British origin) had been maintained in the Dow Chemical Company Laboratory since 1982 without drastic changes in population.
Population maintained at 25C for past 3 years and sustained on Ankistrodesmus convulutus {reared in medium based on Provasoli and Pintner (1968, Ecological implications of in vitro nutritional requirements of algal flagellates", Ann NY Acad. ScL 56, 839-851.) and Nitzschia frustulum Kutzing cultured in ES-I-Si, a medium developed by Provasoli (1968, "Media and prospects for the cultivation of marine algae", in Watanabe A et ai, Cultures and collections of algae, Proceedings of a US-Japan conference, Hakone 1966.) Algal diet axeniC.Test conditions: The. testing conditions followed the basic tenets of the original three-brood test proposed by Mount and Norberg (1984) but were revised in that they emphasize the needs of the animals in terms of space and diet. Details of the conditions may be found in in Cowgill and Milazzo (1989). Test vessels were wide mouth clear glass jars graduated in milliliters to contain 150mL. Into each jar was fitted a glass tube, 3.5 cm diameter.
which had affixed to one end a nytex screen of 243 !-1m mesh for C. dubia or 1000 !-1m mesh for D. magna, These screens were affixed to the glass tubes with silicone glue. After the screens were glued to the glass tubes, three glass beads, 8 mm in diameter, were affixed to the underside equidistant from each other. This was covered with a glass petal dish 5.5 cm in diameter. The jar containing the screened tube was filled with double distilled water and autoclaved for 10 mins at a pressure of 124 kPa. This procedure was repeated three times, renewing the distilled water each time, before the equipment was used for a test.
This procedure accomplished the complete removal of all effects of the silicone glue. Only glass vessels were used.

Remark Results based on total progeny EC5026mg/1 (95% CI 0.5-1443) NOEL 9.6mg/1 Results based on number of broods EC50 38mgll (95% CI 0.6-2554) NOEL 16mg/l Results based on mean brood size EC50 33mg/l (95% CI 0.6-1820) NOEL 9.6mg/l

Test Condition Analysis of Lake Huron water used in culturing and testing
Al 140

NH3 total ND(l0)
B 40
Ca 18700
Cr 8
Cu 5
F 80
Fe 17
Pb ND (5)
Mg 7800
Mn ND (5)
K 1040
Si 3400
Na 4800
S 6000
Zn 8
Total dissolved solids 118000
Total suspended solids NA
Total organic carbon 1600
Test conditions Test vessel: Capacity 150ml, Content 100ml Screen composition: Nytex, Screen mesh size 243IJm Light lux: 670 ± 100 lux Photoperiod, 16 h light, 8 h dark Temperature 25 ± 2 Dissolved oxygen, 8.0 ± 1.5mg/L pH: 8.2 ± 0.2 Dilution water Hardness, as mg CaC03,1L: 90-110 Alkalinity, as mg CaC03/L: 55-75 Habitat: Environmental chamber Habitat changing frequency: Every other day Diet: algae (A. convolutes, N. frustulum) Feeding rate (cells/vessel): A. convolutes 9x10"6, N.
frustulum 1.8x10"6 Feeding frequency: daily Age of organisms, <12h (all from fourth brood.) Number of control broods: 3 Permitted control loss, 20% Number of organisms/ vessel: 1 Number of organisms/Concentration: 10 Number of organisms!lcontrol: 20Test length. days: 7-10.
Variables monitored Daily: light. temperature, survival, progeny Variables monitored every second day: water quality variables in renewed solutions.
Variables monitored at Test termination: Survival, total progeny, adult weight Endpoints: Survival, total progeny, dry adult weight, number of broods, mean brood size, loss of control limited to 20% (LC50/EC50/NOEC) Test ended when the control animals had produced three broods.
Test concentrations used: not specified.

Reliability (2) valid with restrictions This is a well reported study, particularly regarding the methodology of testing. The main weakness is lack of detail on test concentrations used and on the analytical method used to assess test substance concentration

Reference Cowgill, U.M., Milazzo, D.P. (1991) The sensitivity of

	Ceriodaphnia dubia and Daphnia magna to Seven Chemicals Utilizing the Three Brood Test. Arch Environ Contam Toxicol 20(2):211-217.
11.11.2004	(125)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Daphnia magna (Crustacea)
Endpoint	Mortality
Exposure period	11 day(s)
Unit	mg/l
NOEC	= 9.6
LC50	=454
Analytical monitoring	no data
Method	other: see freetext
Year	1990
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Follows the basic methodology for the three brood test proposed by Mount and Norberg (Mount, D.J. and Norberg, T.J. (1984) A seven-day life cycle cladoceran toxicity test. Environ. Toxicol. Chem. 3,425 - 434).Analytical methods used for test substance: no data given.Vehicie used: not required.Statistical methods: For LC50: probn, moving average and nonlinear interpolation. Calculation of point estimates and other corresponding 95% confidence intervals made using a program written by Stephan (1977, Methods for calculating an LC50, In Mayer FL et al (eds), Aquatic toxicology and hazard assessment, ASTM STP 634: 65-84). Calculation of EC50: statistical package SAS GLM (1987, SAS/ST A T guide for personal computers, version 6th ed, SAS institute Inc, Cary, NC) used to generate regression equations. NOELs calculated using Dunnett's t-test.Test organism: Daphnia magna strauss 1820 populations (of British origin) had been maintained in the Dow Chemical Company Laboratory since 1982 without drastic changes in population. Population maintained at 25C for past 3 years and sustained on Ankistrodesmus convulutus (reared in medium based on Provasoli and Pintner (1968, Ecological implications of in vitro nutritional requirements of algal flagellates", Ann NY Acad. ScL 56, 839-851.) and Nitzschia frustulum Kutzing cultured in ES-I-Si, a medium developed by Provasoli (1968, "Media and prospects for the cultivation of marine algae". in Watanabe A et ai, Cultures and collections of algae, Proceedings of a US~Japan conference, Hakone 1966.) Algal

	diet axenic. Test conditions: The. testing conditions followed the basic tenets of the original three-brood test proposed by Mount and Norberg (1984) but were revised in that they emphasize the needs of the animals in terms of space and diet. Details of the conditions may be found in in Cowgill and Milazzo (1989). Test vessels were wide mouth clear glass jars graduated in milliliters to contain 150mL. Into each jar was fitted a glass tube, 3.5 cm diameter. which had affixed to one end a nytex screen of 243 IJm mesh for C. dubia or 1000 IJm mesh for D. magna, These screens were affixed to the glass tubes with silicone glue. After the screens were glued to the glass tubes, three glass beads, 8 mm in diameter, were affixed to the underside equidistant from each other. This was covered with a glass petal dish 5.5 cm in diameter. The jar containing the screened tube was filled with double distilled water and autoclaved for 10 mins at a pressure of 124 kPa. This procedure was repeated three times, renewing the distilled water each time, before the equipment was used for a test. This procedure accomplished the complete removal of all effects of the silicone glue. Only glass vessels were used.
Remark	Using the USEPA classification scheme, ethanol would be classified as practically non toxic based on survival. Based on reproductive parameters, it would be classified as slightly toxic. LC50 (48hr) 9248mg/l (95% CI 7560-12600) LC50 (9 day) 454mg/l (95% CI 232-814) NOEL (11 day) 9.6 mg/l
Test Condition	Analysis of Lake Huron water used in culturing and testing Al 105 NH3 total ND(10) B 332 Ca 45050 Cr ND(5) Cu 13 F 75 Fe 12 Pb ND (5) Mg 7600 Mn ND (5) K 2485 Si 4760 Na 5700 S 5585 Zn 15 Total dissolved solids 233500

	Total suspended solids 1125 Total organic carbon 1400 Test conditions Test vessel: Capacity 150ml, Content 100ml Screen composition: Nytex, Screen mesh size 1000l-lm Light lux: 2150 ± 300 lux Photoperiod, 16 h light, 8 h dark Temperature 25 ± 2 Dissolved oxygen, 8.0 ± 1.5mg/l pH: 8.2 ± 0.2 Dilution water Hardness, as mg CaC03,/l: 160-180 Alkalinity, as mg CaC03/L: 40-52 Habitat: Environmental chamber Habitat changing frequency: Every other day Feeding rate (cellslvessel): A. convolutes 18x10"6, N. frustulum 3.6 x10"6 Feeding frequency: daily Age of organisms, <12h (all from fourth brood.) Number of control broods: 3 Permitted control loss, 20% Number of organisms/ vessel: 1 Number of organisms/Concentration: 10 Number of organisms!lcontrol: 20 Test length, days: 9-11 Variables monitored Daily: light, temperature, survival, progeny Variables monitored every second day: water quality variables in renewed solutions Variables monitored at Test termination: Survival, total progeny, adult weightEndpoints: Survival, total progeny, dry adult weight, number of broods, mean brood size, loss of control limited to 20% (lC50/EC50/NOEC) Test ended when the control animals had produced three broods.
Results	Test concentrations used: not specified.
Reliability	(2) valid with restrictions This is a well reported study, particularly regarding the methodology of testing. The main weakness is lack of detail on test concentrations used and on the analytical method used to assess test substance concentration.
Reference	Cowgill, U.M., Milazzo, D.P. (1991) The sensitivity of Ceriodaphnia dubia and Daphnia magna to Seven Chemicals Utilizing the Three Brood Test. Arch Environ Contam Toxicol 20(2):211-217.
11.11.2004	(125)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Daphnia magna (Crustacea)
Endpoint	reproduction rate
Exposure period	11 day(s)
Unit	mg/l
NOEC	= 9.6
EC50	14 - 26
LC50	454
Analytical monitoring	no data
Method	other
Year	1990
GLP	no data

Test substance	95 – 99.9% ethanol (64-17-5)
Method	Follows the basic methodology for the three brood test proposed by Mount and Norberg (Mount, D.J. and Norberg, T.J. (1984) A seven-day life cycle c1adoceran toxicity test. Environ. Toxicol. Chern. 3, 425 - 434).Analytical methods used for test substance: no data given.Vehicle used: not required.Statistical methods: For LC50: Probit, moving average and nonlinear interpolation.. Calculation of point estimates and other corresponding 95% confidence intervals made using a program written by Stephan (1977, Methods for calculating an LC50, In Mayer FL et al (eds), Aquatic toxicology and hazard assessment, ASTM STP 634: 65-84). Calculation of EC50: statistical package SAS GLM (1987, SAS/STAT guide for personal computers, version 6th ed, SAS institute Inc, Cary, NC) used to generate regression equations. NOELs calculated using Dunnett's t-test.Test organism: Daphnia magna strauss 1820 populations (of British origin) had been maintained in the Dow Chemical Company Laboratory since 1982 without drastic changes in population. Population maintained at 25C for past 3 years and sustained on Ankistrodesmus convulutus (reared in medium based on Provasoli and Pintner (1968, Ecological implications of in vitro nutritional requirements of algal flagellates", Ann NY Acad. ScL 56, 839-851.) and Nitzschia frustulum Kutzing cultured in ES-I-Si, a medium developed by Provasoli (1968, "Media and prospects for the cultivation of marine algae", in Watanabe A et ai, Cultures and collections of algae, Proceedings of a US-Japan conference, Hakone 1966.) Algal diet axenicTest conditions: The. testing conditions followed the basic tenets of the original three-brood test proposed by Mount and Norberg (1984) but were revised in that they emphasize the needs of the animals in terms of space and diet. Details of the conditions may be found in in Cowgill and Milazzo (1989). Test vessels were wide mouth clear glass Jars graduated in milliliters to contain 150mL. Into each jar was fitted a glass tube, 3.5 cm diameter. which had affixed to one end a nytex screen of 243 IJm mesh for C. dubia or 1000 IJm mesh for D. magna, These screens were affixed to the glass tubes with silicone glue. After the screens were glued to the glass tubes, three glass beads, 8 mm in diameter, were affixed to the underside equidistant from each other. This was covered with a glass petal dish 5.5 cm in diameter. The jar containing the screened tube was filled with double distilled water and autoclaved for 10 mins at a pressure of 124 kPa. This procedure was repeated three times, renewing the distilled water each time, before the equipment was used for

	a test. This procedure accomplished the complete removal of all effects of the silicone glue. Only glass vessels were used.
Remark	Using the USEPA classification scheme, ethanol would be classified as practically non toxic based on survival. Based on reproductive parameters, it would be classified as slightly toxic.
Results	Results based on total progeny EC50 14mgfl (95% Cl 0.8-274) NOEL 9.6mg/1 Results based on number of broods EC50 26mgfl (95% CI1-640) NOEL 16mgfl Results based on mean brood size EC50 15mg/1 (95% CI 0.9-278) NOEL 9.6mg/J
Test Condition	Analysis of Lake Huron water used in culturing and testing Al 105 NH3 total ND(l0) B 332 Ca 45050 Cr ND(5) Cu 13 F 75 Fe 12 Pb ND (5) Mg 7600 Mn ND (5) K 2485 Si 4760 Na 5700 S 5585 Zn 15 Total dissolved solids 233500 Total suspended solids 1125 Total organic carbon 1400 Test conditions Test vessel: Capacity 150ml, Content100ml Screen composition: Nytex, Screen mesh size 1000 µm Light lux: 2150 ± 300 lux Photoperiod, 16 h light, 8 h dark Temperature 25 ± 2 Dissolved oxygen, 8.0 ± 1.5mg/L pH: 8.2 ± 0.2 Dilution water Hardness, as mg CaC03,/L: 160-180 Alkalinity, as mg CaC03/L: 40-52 Habitat: Environmental chamber Habitat changing frequency: Every other day Feeding rate (cells/vessel): A. convolutes 18x10A6, N. frustulum 3.6 x1 O^6 Feeding frequency: daily Age of organisms, <12h (all from fourth brood.)

	Number of control broods: 3 Permitted control loss, 20% Number of organisms/ vessel: 1 Number of organisms/Concentration: 10 Number of organisms/control: 20 Test length, days: 9-11 Variables monitored Daily: light, temperature, survival, progeny Variables monitored every second day: water quality variables in renewed solutions Variables monitored at Test termination: Survival, total progeny, adult weight Endpoints: Survival, total progeny, dry adult weight, number of broods, mean brood size, loss of control limited to 20% (LC50/EC50/NOEC) Test ended when the control animals had produced three broods. Test concentrations used: not specified.
Reliability	(2) valid with restrictions
Reference	Cowgill, U.M., Milazzo, D.P. (1991) The sensitivity of Ceriodaphnia dubia and Daphnia magna to Seven Chemicals Utilizing the Three Brood Test. Arch Environ Contam Toxicol 20(2):211-217.
11.11.2004	(125)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Palaemonetes pugio (Crustacea)
Endpoint	other: embryo aute toxicity
Exposure period	12 day(s)
Unit	g/l
LC50	= 3 - 4.5
Analytical monitoring	no data
Method	other: see freetext
Year	1995
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Adult male and female grass shrimp were collected by dip net during spring and autumn 1995 from relatively uncontaminated local estuaries near the U. S. Environmental Protection Agency. Gulf Ecology Division. Gulf Breeze, Florida. The grass shrimp were placed in ice chests with water from the collection site, transported to the laboratory. The grass shrimp were acclimated slowly to 251 and 20-ppt salinity over a 4-h period and were maintained communally in glass aquaria with flow-through

	seawater at 250C and20-ppt salinity. Adult grass shrintp were held in the aquaria for at least two weeks before use. For each test, gravid female grass shrimp were examined with a dissecting microscope for presence of embryos in the tissue cap stage (2-3 dafter oviposition. Female grass shrimp with embryos at the tissue-cap stage were placed under a dissecting microscope and the embryos gently removed from female pleopods and separated from other embryos using forceps and fine-tip probes. Separated embryos were washed three times in filtered 20-ppt seawater.SEATOX, a 4-d test protocol, was used as a screening test that extended from 2-3 d prior to hatch through the hatching period (Rayburn 1996, Characterisation of grass shrimp embryotoxicity test using the water soluble fraction of no 2 fuel oil. Mar Poll Bull, 32(12) 860-8). Embryos at the tissue cap stage (3 dafter Oviposition were collected and placed individually into wells of 24-well plastic tissue culture plates. These were placed into an incubator at 27C and gently rotated at 60rpm. Six days later (9d after oviposition) the embryos were removed and re-examined microscopically. Normal embryos exhibited well developed eyes, a beating heart and visible limbs. Dead or abnormal embryos were discarded and replaced with normal embryos from excess plates kept in the same conditions. Plates of embryos were then randomly selected for a given exposure concentration and the seawater was removed and replaced with 2 ml of test solution. Plates were returned to the 27C incubators and examined daily for mortalities and hatching. The test was terminated after a 4-d exposure, 13d after oviposition. Three tests were performed with 5-6 solvent different concentrations (no further data).Statistical analysis: LC50s with confidence intervals were calculated by Litchfield-Wilcoxon probit analysis.
Remark	The overall control mortality was 7.4% (16/216).
Result	LC50 (4 day) average 12.07g/1 (of three replicates, values 12.39, 12.15, 11.6). The mortality curve was extremely sharp and demonstrated a linear concentration response curve.LC50 (12 day) average 3.63g/l (of three replicates, values 4.5, 3,31, 3.00). The range of concentrations over which mortality occured was much broader that with the 4 day test.
Reliability	(2) valid with restrictions
Reference	Rayburn, J.R., Fisher, W.S. Developmental toxicity of three carrier solvents using embryos of the grass shrimp, Palaemonetes pugio. Arch Environ Contam Toxicol. 1997;33(2):217221.
20.09.2003	(126)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Palaemonetes pugio (Crustacea)
Endpoint	other: embryo teratogenesis
Exposure period	12 day(s)
Unit	g/l
NOEC	>.079
LOEC	=.39
Analytical monitoring	no data
Method	other: see freetext
Year	1995
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)

Method

Adult male and female grass shrimp were collected by dip net during spring and autumn 1995 from relatively uncontaminated local estuaries near the U. S. Environmental Protection Agency. Gulf Ecology Division. Gulf Breeze, Florida. The grass shrimp were placed in ice chests with water from the collection site, transported to the laboratory. The grass shrimp were acclimated slowly to 251 and 20-ppt salinity over a 4-h period and were maintained communally in glass aquaria with flow-through seawater at 250C and 20-ppt salinity. Adult grass shrimp were held in the aquaria for at least two weeks before use. For each test, gravid female grass shrimp were examined with a dissecting microscope for presence of embryos in the tissue cap stage (2-3 dafter oviposition. Female grass shrimp with embryos at the tissue-cap stage were placed under a dissecting microscope and the embryos gently removed from female pleopods and separated from other embryos using forceps and fine-tip probes. Separated embryos were washed three times in filtered 20-ppt seawater.Three·12-d tests were performed according to Rayburn (Rayburn 1996, Characterisation of grass shrimp embryotoxicity test using the water soluble fraction of no 2 fuel all. Mar Poll Bull, 32(12) 860-8) using 24-well plastic tissue culture plates for each solvent tested. Each well contained a single embryo and 2 ml of test solution (static). Each treatment dilution or control was conducted within a single 24-well tissue culture plate N = 24). Plates were placed on rotary shakers (60 rpm) in incubators in the dark and kept at 27 ± IC. Plates were removed from the incubator daily and each embryo was examined for abnormalities of the eye, yolk, heart, head, hepatopancreas, and telson. Both the number and type of abnormality were recorded. Survival was determined by structural integrity of the embryo during the first four days of

	the test, and thereafter by the presence or absence of heartbeat. Mortalities and hatching were recorded daily. Exposures were terminated after 12 d(14-15 d after oviposition). Three tests were conducted. LC50 values with 95% confidence intervals and coefficients of variation were calculated from total mortalities.Treatment concentrations: 0.079,0.39,0.79,1.97,3.95,7.9 g/l. Statistical analysis: LC50s with confidence intervals were calculated by Litchfield-Wilcoxon probit analysis.
Remark	The overall; control mortality was 7.4% (16/216). Developmental abnormalities were not noted at the 0.079g/1 concentration but were seen at 0.39 and 0.79gll and resulted in delayed hatching. Two embryos failed to hatch properly and had swimming difficulties as larvae. Malformations were detected in 21.7% of the embryos exposed to the 3 lowest concentrations and most of the malformed embryos died before the end of the assay. Developmental delay was detected 6 days after oviposition at the three highers concentrations. By 9 days nearly all the embryos exposed to the highest concentration died before the end of the assay and all embryos that died were malformed before the died. Only the 1.97g/1 treatments had larvae that survived with malformations.
Reliability	(2) valid with restrictions
Reference	Rayburn, J.R., Fisher, W.S. Developmental toxicity of three carrier solvents using embryos of the grass shrimp, Palaemonetes pugio. Arch Environ Contam Toxicol 1997;33(2):217221.
11.11.2004	(126)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Palaemonetes pugio (Crustacea)
Endpoint	Mortality
Exposure period	12 day(s)
Unit	mg/l
LOEC	= 2000 - 9100
Analytical monitoring	no data
Method	other
Year	1997
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Adult male and female grass shrimps were collected using push nets from a site in Escambia Bay, Pensacola, Florida. Collections were made in the months of Sept. 1995. March

1996, and May 1996. For the Sept 1995 collection, 70 gravid females and 60 males were collected during high tide. Water temperature was 28.3C and salinity was 20 ppt. For the March 1995 collection, 180 non-gravid females and 150 males were collected during low tide. Water temperature was 16.80 C and salinity was 8 ppt. For the final collection in May 1996, 200 gravid females and 200 males were collected during high tide. Water temperature was 28.1 C and salinity was 3 ppt. Shrimp were placed into coolers filled with site water, transported to the Gulf Ecology Division Laboratory, Gulf Breeze, FL, and identified as Palaemonetes pugio (Williams 1984). Approximately 60 female and 40 male shrimp from each of three collections were transferred into f1owthrough aquaria (80 L) and maintained on a flow rate of- 24L per hour, salinity of 19-22 ppt, and temperature of 19-25C for approximately a sixmonth period. Protective habitats were not furnished in the aquaria. Under these laboratory conditions, the shrimp were able to reproduce and supply adequate numbers of embryos for experiments described here and elsewhere (Little 1968). Shrimp were fed - 2.5 grams of flake food (Tetramin R) daily and twice a week with 25 ml of concentrated brine shrimp (Artemia saline) nauplii.

Experiments were conducted with over a 9 month period using embryos from shrimp that had been maintained in aquaria for different periods of time, from 1-160 days. A single gravid female shrimp with a clutch of embryos 3-d (after oviposition) was selected for testing. Embryos were removed from the female, placed in disposable 24-well flat bottom plastic culture prates and individually exposed to 2 ml of ethanol at five different dilutions (0.05, 0.10, 0.50, 1.0 and 2.0% v/v%) based on 12-d LC50 values from Rayburn and Fisher (1996). Dilutions were made with histological grade 100% EtOH and 20 ppt 0.22 pm filtered natural sea water. Filtered sea water was also used as control. Embryos were placed on rotators (Model G2, New Brunswick Scientific Co.) in an incubator maintained at 2700±1 for 12 d. Rotators were set at 60 rpm to provide a gentle agitation of the embryos in the test wells. After a 12-d exposure, embryos were examined for mortality. 12-d LC50 values and 95% confidence intervals (CI) were calculated using the trimmed SpearmanKarber method (Hamilton et al. 1977). Average of mean 1 2-d LC50 values and coefficients of variation (CV) were calculated according to Steel and Torrie (1980).

Result

Five LC50s were determined from the Sept collection over a

	period from 30-160 days from collection, Four LC50s from the March collection (2-60 days) and two LC50s from the May collection (1-30 days.) 11 tests performed in total in saltwater solutions containing 0.37% to 1.10% vlv ethanol. Average control mortality 11.7% with a standard error of 3.2%. Three results showed mortalities over 16.7%. One results produced a very low value (order of magnitude lower. High control mortality was observed and it was not possible to calculate an LC50. The average value from the remainder was an LC50 value 0.53% (4.18g/l) SD=0.20% (1.58g/l). Embryos oviposited in the field had greater sensitivity (2-10x) than those ovipositied in the laboratory.
Reliability	(2) valid with restrictions
Reference	Foss, S.S, Rayburn, J.R. Effects of culture duration on toxicity of ethanol to developing embryos of the grass shrimp Palaeomonetes pugio. Bull Environ Contam Toxicol 1997; 59: 467-471.
11.11.2004	(127)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	other aquatic crustacea
Endpoint	Mortality
Exposure period	28 day(s)
Unit	mmol/l = 25 - 150
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Behaviour = 25 mmol; Growth = 150 mmol; Mortality = 75-150 mmol.
Reliability	(4) not assignable
Reference	Friedman, R.N., Bittner, G.D., Blundon, J.A. Electrophysiological and behavioural effects of ethanol on crayfish. J Pharmacol Exp Ther 1988; 246 (1):125-131.
05.10.2003	(128)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	other aquatic crustacea
Endpoint	Mortality
Exposure period	56 day(s)
Analytical monitoring	no data

Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Reliability	(4) not assignable This otherwise robust study of the acute and chronic toxicity of pentachlorophenol In 95% ethanol referred to a 'solvent control' but the concentration of ethanol was not given. nor was a median lethal concentration determined for the solvent control. Mortality rate in controls was high for Calamoecia lucasi sublethal tests because of the difficulties experienced in their culture.
Reference	Willis, K.J. Acute and chronic bioassays with New Zealand freshwater copepods using pentachlorophenol. Environ Toxicol Chem 1999; 18 (11): 2580-2586
05.10.2003	(129)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	other aquatic mollusc: littorina littorea
Endpoint	other: morphological changes (imposex)
Analytical monitoring	no data
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	The study was primarily on the effects of tributyl tin, Pb and Sn. Ethanol only controls received 50 or 100 ng/l. Ethanol significantly increased length of penis confounding the interpretation of the effects of heavy metal compounds.
Reliability	(4) not assignable
Reference	Deutsch, U., Gehlmann, J.; Stroben, E. Morphological effectsof tributyl tin (TBT) in vitro on the genital system of the Mesogastropod Littorina littorea (l.)(Prosobranchia) In: J. C. Aldrich (Ed.), Proc 27th European Marine Biology Symposium, Quantified Phenotypic Responses in Morphology and Physiology, Sept. 7-11, 1992, Dublin, Ireland: 297-300.
22.09.2003	(130)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance:	1-butanol (71-36-3)
Value:	21 mg/L
Remark:	A chronic daphnid 16-d LC50 was calculated using ECOSAR, from the USEP A. The preferred physical properties were used.

The SAR for esters was employed. The structure was determined from the CAS RN as stored in the accompanying database of SMILES notations within ECOSAR. Chemicalspecific input parameters were: molecular weight (74.12 g/mol), vapor pressure (0.56 hPa or 0.42 mm Hg), log Kow (0.88), melting point -89.9° C, aqueous solubility 77,000 mglL, boiling point of 117.6° C, and a Henry's Law constant of 5.3 E7 atm-m3/mol.

Reliability: (2) valid with restriction, calculated value

Reference: EPA's ECOSAR model (v. 0.991). EPISUITE v.3.l0, U.S. Environmental Protection Agency, April (2001).

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: Daphnia magna (Crustacea)
Endpoint: other: Survival, growth and reproduction rate
Exposure period: 21 day(s)
Unit: mg/l **Analytical monitoring:**
NOEC: = 6.8 - 13 calculated

Method: other: calculated (QSAR)
Year: 2005
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Method: Measured data of an acceptable quality are available for 21-day reproduction studies with Daphnia magna for the single carbon chain length alcohols 1-octanol (111-87-5), 1-decanol (112-30-1), 1-dodecanol (112-53-8; supporting), 1-tetradecanol (112-72-1) and 1-pentadecanol (629-76-5). The studies are described in the relevant dossiers and in Annex X to the SIAR. The data were obtained generally in accordance with standard test guideline OECD 211. No measured data are available for mixtures of different carbon chain length alcohols.

The data suggest that for substances of chain length greater than C15, no chronic effects would be expected.

Structure-activity relationships have been developed based on these results. It is possible to apply these structure-activity relationships to estimate chronic toxicity endpoints where there are no reliable measured data.

Two QSAR relationships have been developed. It can be concluded that the NOEC for reproduction would be within the range of the two estimates.

Result: It can be estimated that chronic NOEC(reproduction) for Daphnia magna would lie in the range of 6.8 - 13.0 mg/l.
Reliability: (2) valid with restrictions
Value estimated based on findings for similar substances (other Category members) in reliable studies.
Flag: Critical study for SIDS endpoint
Reference: Annex X (2005). Chronic Toxicity of Long Chain Alcohols to Daphnia magna; Annex X to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (5)

<u>1-Octanol (111-87-5) for 1-Octanol Aluminum Salt (14624-13-6)</u>

Species: Daphnia magna (Crustacea)
Endpoint: other: Mortality, reproduction rate, and appearance of offspring
Exposure period: 21 day(s)
Unit: mg/l
Analytical monitoring: no
NOEC: = 1

Method: other
Year: 1988
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Method: Recommendation of the German Federal Environmental Agency on the Performance of Testing according to Sec 5, Para 1, No. 3 of the Regulation on Application Documents and Evidence under the Chemicals Act.
Remark: Primarily, the results were expressed with reference to the nominal concentration. If however, the chemical analysis showed a loss of tested substance greater than 20% , then the lowest analysed concentration (minimum value) obtained during the test was also given for the NOEC.
The 21-d NOEC based on nominal concentrations was 1.6 mg/l.
The 21-d NOEC based on the minimum value for 1-Octanol was 1.0 mg/l.
Result: RESULTS: EXPOSED
21d NOEC = 1.6 mg/l (based on nominal value)
21d NOEC = 1.0 mg/l (based on measured value)
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
Test condition: TEST ORGANISMS
Strain: Daphnia magna
Supplier: Laboratory culture

Age: 24 hours old
Feeding: Tetramin-Hauptfutter (fish feed) and activated sludge were used as feeds, daphnia fed daily.
Control group: 1 control group (4 replicates, five animals per replicate)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle/solvent: none
DILUTION WATER
Source: Deionised water
Aeration: Aerated up to the water saturation level
Alkalinity: not reported
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: 0.4 to 50 mg/l
Renewal of test solution: Parent animals in test and control vessels were pipetted 3 times a week (Mondays, Wednesdays and Fridays) into freshly prepared test and control media
Exposure vessel type: 400 ml beakers
Number of replicates: 4 per concentration
Animals per replicate: 5
Test temperature: 25 +/- 1 degree C
Dissolved oxygen: Average minimum oxygen saturation value of 69% was measured at the end of the test period (related to all test substances in test)
pH mean: >7
TEST PARAMETER: mortality, reproduction rate and appearance of offspring
MONITORING OF TEST SUBSTANCE CONCENTRATION: Samples were taken twice from selected concentration levels of the test series during the test period and analysed chemically.

Reliability: (2) valid with restrictions
Best study although not a SIDS endpoint.

Reference: Kuhn, R., Pattard, M., Pernak, K., and Winter, A. 1989. Results of the harmful effects of water pollutants to Daphnia magna in the 21 day reproduction test. Wat. Res. 23 (4): 501-510.

19-JUL-2005 (75)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Species: Daphnia magna (Crustacea)
Endpoint: other: Survival, growth and reproduction rate
Exposure period: 21 day(s)
Unit: µg/l

Analytical monitoring: yes
NOEC: = 110 measured/nominal
LOEC: = 370 measured/nominal
EC10 : = 210 measured/nominal

Method: OECD Guide-line 211
Year: 2005
GLP: yes
Test substance: > 90% 1-decanol (112-30-1)

Method: GUIDELINE: OECD 211 with modifications to allow aeration of exposure media.

STATISTICS: The evaluation of the concentration-effect-relationships and the calculations of effect concentrations were based on mean measured initial concentrations as multiple peak concentrations, as well as on geometric means between mean measured initial and aged (24h) test concentrations. For each endpoint, the NOEC, LOEC, and, if possible, the EC50, EC20 and EC10 were determined. A LOEC and NOEC were calculated by ANOVA followed by Williams' test or an appropriate non-parametric test suggested by the ToxRat program. When the test results showed a concentration-response relationship, the data were analysed by regression using Probit-analysis assuming log-normal distribution of the values using the computer program ToxRat program.

TEST CONCENTRATIONS: Nominal test concentrations were 0, 152, 411, 1110 and 3000 µg test item/L. Initial mean measured concentrations of freshly prepared test solutions were 1.6, 122, 351, 962, 2800 µg/L. Geometric means of mean measured initial and aged concentrations after 24 h hours were <LOQ, 23.3, 107, 367 and 1227 µg/L.

TEST MEDIUM PREPARATION: Test solutions were prepared daily by stirring the test substance in test media under slow stir conditions (21 h) in sterilized mixing vessels. The mixing vessels were cylindrical brown glass bottles with teflon covered screw caps, fitted with a drain port near the bottom for drawing off the test solution. The volume of the mixing vessels was 2 L. After stirring, the contents of the vessels were left to settle for 2 h. The saturated aqueous phase was then taken out of the drain port. The first fraction 0-100 mL was withdrawn. The fraction between 100 and 1800 mL was used for rinsing (200 mL) and filling (1000 mL) the test flasks for toxicity testing and for analytical measurements (500 mL), if

done. Rinsing of the test vessels was carried out to saturate the surfaces of the test vessels. After filling, the vessels were closed immediately by using autoclaved silicone stoppers and only opened to introduce the test organisms and again at the renewals of the test media. The test media were not stored for more than 1 - 2 hours prior to testing

EXPOSURE REGIME: Semi-static, daily renewal. As a deviation from OECD Guideline 211, all test vessels were aerated with sterile filtrated synthetic air: the autoclaved silicone stoppers were fitted with fine glass capillaries connected to the aeration unit. The aeration was necessary to avoid severe oxygen depletion due to the increase of transferred bacteria with growing Daphnia magna as observed in pre-studies and the associated oxygen consumption by the degradation of the test substance.

TEST ORGANISMS: Daphnia magna STRAUS, Crustacea, Cladocera. Age: 4 - 24 hours old. Origin: Umweltbundesamt (German Federal Environment Agency). Test organisms bred in the laboratory of the Fh-IME (testing facility).

TEST APPARATUS: Each Daphnia magna was exposed separately in a numbered vessel flask) containing 100 mL of test medium.

FEEDING: The Daphnia magna were fed at each renewal with suspensions of unicellular green algae. The suspensions of Desmodesmus subspicatus (daily prepared from axenic cultures) were controlled analyzed for microbial contamination one and two weeks after test start by using "Cult-Dip combi® Dip Slides (Merck)". No bacterial contamination was detected. The content of food in the test suspensions, measured as turbidity at 758 nm, increased during the test from 7 mg C/L equivalents to 15 mg C/L equivalents.

TEST DESIGN: For each test concentration and for the control 10x1 animals were used.

TEST CONDITIONS: The vessels were subjected to a light/dark cycle of 16/8 hours. The test temperature during the test was in the range 20.0 to 21.0°C, the light intensity was in the range 588 to 657 lux. The oxygen saturation never fell below 70 % (5.7 mg/L), and the mean pH was 9.4 to 9.5 at all treatment levels.

ENDPOINT OBSERVATIONS: The parent Daphnia magna were assessed

visually daily for immobility and any other abnormalities in appearance and behaviour. At study termination, the length of the adults was measured by digital photography and image analysis and their statistics compared with those of the control animals. The newborn Daphnia magna in each beaker were

counted at each daily renewal of the test solutions, inspected for abnormalities in condition, and removed. The following endpoints observed in the reproduction test were evaluated quantitatively:
o Mortality (immobility) of parental generation Daphnia magna
o Age at first brood
o Total number of offspring per replicate
o Cumulative Number of live offspring per surviving female at the time of recording
o Intrinsic rate of increase, r
o Individual length of adults

ANALYSIS OF TEST MEDIA: All the test concentrations were sampled for chemical analysis three times a week at renewal of the test media. A 500 mL aliquot of the fresh solutions was used for analysis. After 24 h, at the next renewal, the aged test liquids were pooled (vessels 1- 5 and 6-10) and analysed. The analyte was extracted from the aqueous test samples by liquid-liquid partitioning with n-hexane. After derivatization of the analyte by MSTFA measurement was performed by GC-MS using n-dodecanol-d25 as internal standard. The method was validated for the determination of the test item in Daphnia test medium in the concentration range of 1.0 - 100 µg/L

Result: SURVIVAL, GROWTH AND REPRODUCTION DATA

Test item Nominal conc. (µg/L)	Survival (%)	Growth (length) Mean ± SD (mm)	Age at first brood Mean ± SD (days)
Control	100	5.41 ± 0.22	8.9 ± 0.74
152	100	5.52 ± 0.19	9.2 ± 0.79
411	100	5.43 ± 0.21	9.0 ± 0.82
1110	100	5.26 ± 0.38	9.4 ± 0.97
3000	0	n.d.	n.d.

Test item nominal conc. (µg/L)	Cumulative offspring per female Mean ± SD (#)	Intrinsic rate of increase r Mean ± SD (1/d)
Control	68.1 ± 9.5	0.294 ± 0.017

152	68.0 ± 5.6	0.297 ± 0.018
411	62.9 ± 5.8	0.281 ± 0.011
1110	58.6 ± 7.7 *	0.277 ± 0.024 *
3000	n.d.	n.d

* significant difference to control according Williams-test (a = 0.05, one-sided smaller)

CALCULATED STATISTICS:

Related to daily initial concentrations:
EC10 = 610 µg test item/L
EC20 = 1500 µg test item/L
LOEC = 960 µg test item/L
NOEC = 350 µg test item/L

Related to mean measured concentrations:
EC10 = 210 µg test item/L
EC20 = 670 µg test item/L
LOEC = 370 µg test item/L
NOEC = 110 µg test item/L

Test substance: C10 Fatty alcohol (1-Decanol)
CAS No. 112-30-1
Sample received from Laboratory Dr. Ehrenstorfer-Schafers, Augsburg, Germany.
Lot No: 21011
Purity: 99.5 % ± 0.5 %

Reliability: (1) valid without restriction
Guideline study conducted in accordance with GLP.

Flag: Critical study for SIDS endpoint

Reference: Schafers, C. (2005). Daphnia magna, reproduction test in closed vessels following OECD 211. C10 fatty alcohol. GLP code: SDA-005/4-21. Fraunhofer Institute for Molecular Biology and Applied Ecology (IME) 57377 Schmallenberg, Germany.

04-NOV-2005 (76)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)</u>

Species: Daphnia magna (Crustacea)
Endpoint: Survival, growth and reproduction rate
Exposure period: 21 day(s)
Unit: ug/l
Analytical monitoring: yes
NOEC: 14
LOEC: 95

EC10: 13
EC20: 34

Method: OECD 211
Year: 2005
GLP: yes
Test substance: other TS: Dodecanol (112-53-8)

Method:
GUIDELINE: OECD 211 with modifications to allow aeration of exposure media.

STATISTICS: The evaluation of the concentration-effect-relationships and the calculations of effect concentrations were based on mean measured initial concentrations as multiple peak concentrations, as well as on geometric means between mean measured initial and aged (24h) test concentrations. For each endpoint, the NOEC, LOEC, and, if possible, the EC50, EC20 and EC10 were determined. A LOEC and NOEC were calculated by ANOVA followed by Williams' test or an appropriate non-parametric test suggested by the ToxRat program. When the test results showed a concentration-response relationship, the data were analysed by regression using Probit-analysis assuming log-normal distribution of the values using the computer program ToxRat program.

TEST CONCENTRATIONS: Nominal test concentrations were 0, 25, 69, 185 and 500 µg test item/L. Mean measured concentrations of freshly prepared test solutions were <Limit of quantification, 20, 56, 163 and 534 µg/L. The geometric means of mean measured initial and aged concentrations after 24 h hours were <Limit of quantification, 3, 5, 14 and 95 µg/L.

TEST MEDIUM PREPARATION: Test solutions were prepared daily by stirring the test substance in test media under slow stir conditions (21 h) in sterilized mixing vessels. The mixing vessels were cylindrical brown glass bottles with teflon covered screw caps, fitted with a drain port near the bottom for drawing off the test solution. The volume of the mixing vessels was 2 L. After stirring, the contents of the vessels were left to settle for 2 h. The saturated aqueous phase was then taken out of the drain port. The first fraction 0-100 mL was discarded. The fraction between 100 and 1800 mL was used for rinsing (200 mL) and filling (1000 mL) the test flasks for toxicity testing and for analytical measurements (500 mL), if done. Rinsing of the test vessels was carried out to saturate the surfaces of the test vessels. After filling, the vessels were closed immediately by using autoclaved silicone stoppers and only opened to introduce the test organisms and again at the renewals of the test media. The test media were not stored for more than 1 - 2 hours prior to testing

EXPOSURE REGIME: Semi-static, daily renewal. As a deviation from OECD Guideline 211, all test vessels were aerated with sterile filtrated synthetic air: the autoclaved silicone stoppers were fitted with fine glass capillaries connected to the aeration unit. The aeration was necessary to avoid severe oxygen depletion due to the increase of transferred bacteria with growing Daphnia magna as observed in pre-studies and the associated oxygen consumption by the degradation of the test substance.

TEST ORGANISMS: *Daphnia magna* STRAUS, Crustacea, Cladocera. Age: 4 - 24 hours old. Origin: Umweltbundesamt (German Federal
Environment Agency). Test organisms bred in the laboratory of the Fh-IME (testing facility).

TEST APPARATUS: Each *Daphnia magna* was exposed separately in a numbered vessel flask) containing 100 mL of test medium.

FEEDING: The *Daphnia magna* were fed at each renewal with suspensions of unicellular green algae. The suspensions of *Desmodesmus subspicatus* (daily prepared from axenic cultures) were controlled analyzed for microbial contamination one and two weeks after test start by using "Cult-Dip combi® Dip Slides (Merck)". No bacterial contamination was detected. The content of food in the test suspensions, measured as turbidity at 758 nm, increased during the test from 7 mg C/L equivalents to
15 mg C/L equivalents.

TEST DESIGN: For each test concentration and for the control 10x1 animals were used.

TEST CONDITIONS: The vessels were subjected to a light/dark cycle of 16/8 hours. The test temperature during the test was in the range 21.0 to 22.0°C, the light intensity was in the range 585 to 647 lux. The oxygen saturation never fell below 56 % (4.0 mg/L), and the mean pH was 9.3 to 9.5 at all treatment levels.

ENDPOINT OBSERVATIONS: The parent *Daphnia magna* were assessed visually daily for immobility and any other abnormalities in appearance and behaviour. At study termination, the length of the adults was measured by digital photography and image analysis and their statistics compared with those of the control animals. The newborn *Daphnia magna* in each beaker were counted at each daily renewal of the test solutions, inspected for abnormalities in condition, and removed. The following endpoints observed in the reproduction test were evaluated quantitatively:

- Mortality (immobility) of parental generation *Daphnia magna*
- Age at first brood
- Total number of offspring per replicate

• Cumulative Number of live offspring per surviving female at the time of recording
• Intrinsic rate of increase, r
• Individual length of adults

ANALYSIS OF TEST MEDIA: All the test concentrations were sampled for chemical analysis three times a week at renewal of the test media. A 500 mL aliquot of the fresh solutions was used for analysis. After 24 h, at the next renewal, the aged test liquids were pooled (vessels 1- 5 and 6-10) and analysed. The analyte was extracted from the aqueous test samples by liquid-liquid partitioning with n-hexane. After derivatization of the analyte by MSTFA measurement was performed by GC-MS using n-dodecanol-d25 as internal standard. The method was validated for the determination of the test item in *Daphnia* test medium in the concentration range of 1.0 - 100 µg/L

Result:

SURVIVAL, GROWTH AND REPRODUCTION DATA

Test item nominal conc. (µg/L)	Survival (%)	Growth (length) Mean ± SD (mm)	Age at first brood Mean ± SD (days)
Test item nominal conc. (µg/L)	Survival (%)	Growth (length) Mean ± SD (mm)	Age at first brood Mean ± SD (days)
Control	100	4.83 ± 0.35	8.2 ± 0.79
25	100	4.37 ± 0.39	8.2 ± 0.92
69	100	4.47 ± 0.31	8.4 ± 0.84
185	100	4.38 ± 0.41	8.1 ± 0.99
500	40	4.76 ± 0.40	8.6 ± 1.14

Test item nominal conc. (µg/L)	Cumulative offspring per female Mean ± SD (#)	Intrinsic rate of increase r Mean ± SD (1/d))
Control	68.0 ± 8.9	0.320 ± 0.024
25	68.0 ± 11.6	0.319 ± 0.026
69	63.0 ± 9.8	0.307 ± 0.018
185	61.0 ± 7.1	0.304 ± 0.019
500	64.0 ± 19.3	0.256 ± 0.044

CALCULATED STATISTICS:

Related to daily initial concentrations:
EC10 = 150 µg test item/L
EC20 = 520 µg test item/L
LOEC = 530 µg test item/L
NOEC = 160 µg test item/L

Related to mean measured concentrations:
EC10 = 13 µg test item/L
EC20 = 34 µg test item/L
LOEC = 95 µg test item/L
NOEC = 14 µg test item/L

Test substance:
C12 Fatty alcohol (1-Dodecanol)
CAS No. 112-53-8
Sample received from Laboratory Dr. Ehrenstorfer-Schafers, Augsburg, Germany.
Lot No: 30403
Purity: 98.0 % ± 0.5 %

Reliability: (1) Reliable without restrictions
Guideline study conducted in accordance with GLP.
Critical Study for SIDS endpoint
Reference: Schafers, C. (2005). Daphnia magna, reproduction test in closed vessels following OECD 211. C12 fatty alcohol. GLP code: SDA-001/4-21. Fraunhofer Institute for Molecular Biology and Applied Ecology (IME) 57377 Schmallenberg, Germany.
(18)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)

Species: Daphnia magna (Crustacea)
Endpoint: other: reproduction rate and mortality
Exposure period: 21 day(s)
Unit: mg/l
Analytical monitoring: yes
NOEC: = 1
LOEC: = 3

Method: other: Comparable to OECD guideline 202, Part 2.
Year: 1992
GLP: yes
Test substance: other TS: Dodecanol (112-53-8)

Method: Chronic toxicity testing in Daphnia magna according to UBA toxicity testing protocol 'Prolonged toxicity test with Daphnia Magna', 01.02.1984; determination of the NOEC for

reproduction rate, mortality and the moment of the first appearance of descendants.

Remark: Data refers to both mortality of parents and number of offspring/parent. The test substance was added directly, without the use of solvents. The aqueous solubility of Dodecanol is 3 mg/l. Effects of mortality were all seen in dose groups above the limit of saturation.

Result: RESULTS:

Concentration (mg/L)	0	1	3	10	30	100
First day of offspring	9-12	9-12	9-12	9-12	9-12	9-12
Survival rate of adults (%)	90	90	90	50	45	40
Average number of young animal per adult	106	112	84	55	25	28
Standard deviation	3.6	3.5	13.2	15.3	12.6	4.3
Significant ($p<0.05$)	--	no	yes	yes	yes	yes

NOEC = 1 mg/L
LOEC = 3 mg/L

CONTROL SUBSTANCE:
No use of control substance reported.

Source: Guhl 1992.

Test condition: TEST ORGANISMS
Strain: Daphnia magna
Supplier: Own breeding, strain is identical with that of BGA
Age: not reported
Feeding: 1 ml algae (1-3* 10E6 cells/ml) and 1 ml activated sludge
Feeding during test: Monday/Wednesday/Friday
Control group: 1 group (4 replicates)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none (test substance was weighed directly into test vessels)
Concentration of vehicle/solvent: not applicable
DILUTION WATER
Source: aerated tap water
Aeration: not reported

Alkalinity: not reported
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: 1, 3, 10, 30 and 100 mg/l
Renewal of test solution: Test solutions changed 3 times per week (Mondays/Wednesdays/Fridays)
Exposure vessel type: 500 ml Erlenmeyer Flasks
Number of replicates: 4
Animals per replicate: 5
Test temperature: 21.5 - 22 C
Dissolved oxygen: 90-92% saturation
pH mean: 8.3-8.5
Intensity of irradiation: Radium 60W
Photoperiod: 16 hours light, 8 hours dark
TEST PARAMETER: reproduction rate and mortality
MONITORING OF TEST SUBSTANCE CONCENTRATION: Measured DOC concentrations at 0, 48 and 120 hours. The mean measured (DOC) concentrations in the 10 mg/l group were 0.55, 1.25 and 1.85 mg/l at 0, 48 and 120 hours respectively. Similar measured concentrations were observed in the 30 and 100 mg/l groups.

Reliability: (2) valid with restrictions

Reference: Guhl, Dr. 1992a. Dodecanol (Lorol C12-99): Bestimmung derchronischen Daphnientoxizitat im verlangerten Daphnian test, 21 Tage. Henkel KGaA Report No. RE 920095.

(5)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-54-8)</u>

Species: other: Brachionus calyciflorus (rotifer)
Endpoint: mortality
Exposure period: 2 day(s)
Unit: mg/l
Analytical monitoring: yes
EC50: = .81 - .88

Method: other
Year: 1996
GLP: no data
Test substance: other TS: Dodecanol (112-53-8)

Method: Test based on modified method of Snell and Moffat (A 2-d life cycle test with the rotifer Brachionus calyciflorus, Environ. Toxicol. Chem. 11:1249-1257 (1992)). Modifications of the diet, water source and light level were

made to better reflect conditions in the natural environment.

Remark: In repeat tests the EC50 values for Dodecanol were 0.81 and 0.88 mg/l.
The 2-day rotifer test is considered a chronic test because multiple broods are produced and the F1 generation produces neonates

Result: RESULTS: EXPOSED
Test 1
EC20 = 0.74 mg/l
EC50 = 0.81 mg/l
Test 2
EC20 = 0.71 mg/l
EC50 = 0.88 mg/l
Based on measured concentrations
RESULTS: CONTROL
Number/percentage of animals showing adverse effects:
Not reported

Source: Versteeg 1997.

Test condition: TEST ORGANISMS
Strain: Brachionus calyciflorus
Supplier: Bioresponse Systems Inc., Halifax, NS, Canada
Age: <3 hours old
Feeding: Algae, Selenastrum capricornutum and Chlorella vulgaris cultured in Bold's basal media were used to feed Rotifers
Pretreatment: Approximately 3000 cysts were hydrated with dilution water 20h prior to test initiation
Feeding during test: Newly hatched swimming rotifers were placed in 10 ml of test water containing an equal mixture of C. vulgaris and S. capricornutum at 1 * 10 6 cells/ml
Control group: 1 control group and solvent group, if appropriate (3 replicates in each)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: not reported
Concentration of vehicle/solvent: not reported
DILUTION WATER
Source: 50/50 blend of locally obtained well water and deionised water
Aeration: not reported
Alkalinity: not reported
Hardness: 152 mg/l $CaCO_3$
Conductance: 450 umhos
TEST SYSTEM
Concentrations: 4-6 test concentrations up to the limit of solubility

Renewal of test solution: none
Exposure vessel type: not reported
Number of replicates: 3
Animals per replicate: 6
Test temperature: 25 +/- 2 C
Dissolved oxygen: 8.5 mg/l
pH mean: 8.6
Adjustment of pH: not reported
Photoperiod: 16/8 h light:dark cycle under low light conditions
TEST PARAMETER: mortality
MONITORING OF TEST SUBSTANCE CONCENTRATION: measured daily, overall test concentrations decreased by 20 to 90% over the 2 day test period, however concentrations for individual compounds not reported.

Reliability: (2) valid with restrictions
Best study although not a SIDS endpoint.

Reference: Versteeg, D.J., Stanton, D.T., Pence, M.A., and Cown, C. 1997. Effects of surfactants on the rotifers, Brachionus calyiflorus, in a chronic toxicity tests and the development of QSARS. Environ. Toxicol. Chem. 16:1051-1058.

25-SEP-2003 (26)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Species: Daphnia magna (Crustacea)
Endpoint: other: Survival, growth and reproduction rate
Exposure period: 21 day(s)
Unit: µg/l
Analytical monitoring: yes
NOEC: = 1.6 measured/nominal
LOEC: = 3.6 measured/nominal
EC10 : = 6.3 measured/nominal

Method: OECD Guide-line 211
Year: 2005
GLP: yes
Test substance: > 95% 1-Tetradecanol (112-72-1)

Method: GUIDELINE: OECD 211 with modifications to allow aeration of exposure media.

STATISTICS: The evaluation of the concentration-effect-relationships and the calculations of effect concentrations were based on mean measured initial concentrations as multiple peak concentrations, as well as on

geometric means between mean measured initial and aged (24h) test concentrations. For each endpoint, the NOEC, LOEC, and, if possible, the EC50, EC20 and EC10 were determined. A LOEC and NOEC were calculated by ANOVA followed by Williams' test or an appropriate non-parametric test suggested by the ToxRat program. When the test results showed a concentration-response relationship, the data were analysed by regression using Probit-analysis assuming log-normal distribution of the values using the computer program ToxRat program.

TEST CONCENTRATIONS: Nominal test concentrations were 0, 24.4, 68.6, 185.2 and 500 µg test item/L. Mean measured concentrations of freshly prepared test solutions were <Limit of quantification, 9.9, 51, 138 and 367 µg/L The geometric means of mean measured initial and aged concentrations after 24 hours were <Limit of quantification, 1.6, 3.6, 13 and 77 µg/L.

TEST MEDIUM PREPARATION: Test solutions were prepared daily by stirring the test substance in test media under slow stir conditions (21 h) in sterilized mixing vessels. The mixing vessels were cylindrical brown glass bottles with teflon covered screw caps, fitted with a drain port near the bottom for drawing off the test solution. The volume of the mixing vessels was 2 L. After stirring, the contents of the vessels were left to settle for 2 h. The saturated aqueous phase was then taken out of the drain port. The first fraction 0-100 mL was withdrawn. The fraction between 100 and 1800 mL was used for rinsing (200 mL) and filling (1000 mL) the test flasks for toxicity testing and for analytical measurements (500 mL), if done. Rinsing of the test vessels was carried out to saturate the surfaces of the test vessels. After filling, the vessels were closed immediately by using autoclaved silicone stoppers and only opened to introduce the test organisms and again at the renewals of the test media. The test media were not stored for more than 1 - 2 hours prior to testing

EXPOSURE REGIME: Semi-static, daily renewal. As a deviation from OECD Guideline 211, all test vessels were aerated with sterile filtrated synthetic air: the autoclaved silicone stoppers were fitted with fine glass capillaries connected to the aeration unit. The aeration was necessary to avoid severe oxygen depletion due to the increase of transferred bacteria with growing Daphnia magna as observed in pre-studies and the associated oxygen consumption by the degradation of the test substance.

TEST ORGANISMS: Daphnia magna STRAUS, Crustacea, Cladocera. Age: 4 - 24 hours old. Origin: Umweltbundesamt (German Federal Environment Agency). Test organisms bred in the laboratory of the Fh-IME (testing facility).

TEST APPARATUS: Each Daphnia magna was exposed separately in a numbered vessel flask) containing 100 mL of test medium.

FEEDING: The Daphnia magna were fed at each renewal with suspensions of unicellular green algae. The suspensions of Desmodesmus subspicatus (daily prepared from axenic cultures) were controlled analyzed for microbial contamination one and two weeks after test start by using "Cult-Dip combi® Dip Slides (Merck)". No bacterial contamination was detected. The content of food in the test suspensions, measured as turbidity at 758 nm, increased during the test from 7 mg C/L equivalents to
15 mg C/L equivalents.

TEST DESIGN: For each test concentration and for the control 10x1 animals were used.

TEST CONDITIONS: The vessels were subjected to a light/dark cycle of 16/8 hours. The test temperature during the test was in the range 20.4 to 21.4°C, the light intensity was in the range 598 to 680 lux. The oxygen saturation never fell below 75 % (6.0 mg/L), and the mean pH was 9.3 to 9.4 at all treatment levels.

ENDPOINT OBSERVATIONS: The parent Daphnia magna were assessed visually daily for immobility and any other abnormalities in appearance and behaviour. At study termination, the length of the adults was measured by digital photography and image analysis and their statistics compared with those of the control animals. The newborn Daphnia magna in each beaker were counted at each daily renewal of the test solutions, inspected for abnormalities in condition, and removed. The following endpoints observed in the reproduction test were evaluated quantitatively:
o Mortality (immobility) of parental generation Daphnia magna
o Age at first brood
o Total number of offspring per replicate
o Cumulative Number of live offspring per surviving female at the time of recording
o Intrinsic rate of increase, r

o Individual length of adults

ANALYSIS OF TEST MEDIA: All the test concentrations were sampled for chemical analysis three times a week at renewal of the test media. A 500 mL aliquot of the fresh solutions was used for analysis. After 24 h, at the next renewal, the aged test liquids were pooled (vessels 1- 5 and 6-10) and analysed. The analyte was extracted from the aqueous test samples by liquid-liquid partitioning with n-hexane. After derivatization of the analyte by MSTFA measurement was performed by GC-MS using n-tetradecanol-d29 as internal standard. The method was validated for the determination of the test item in Daphnia test medium in the concentration range of 0.5 - 100 µg/L.

Result: SURVIVAL, GROWTH AND REPRODUCTION DATA

Test item Nominal conc. (µg/L)	Survival (%)	Growth (length) Mean ± SD (mm)	Age at first brood Mean ± SD (days)
Control	100	4.47 ± 0.32	7.8 ± 0.8
24.4	100	4.83 ± 0.31	7.7 ± 0.7
68.6	100	4.50 ± 0.38	8.1 ± 0.7
185.2	100	4.49 ± 0.27	8.2 ± 0.8
500	70	4.73 ± 0.40	7.9 ± 0.6

Test item nominal conc. (µg/L)	Cumulative offspring per female Mean ± SD (#)	Intrinsic rate of increase r Mean ± SD (1/d)
Control	86.6 ± 5.7	0.368 ± 0.032
24.4	84.0 ± 7.4	0.364 ± 0.034
68.6	79.7 ± 9.4	0.347 ± 0.033
185.2	73.9 ± 8.5	0.338 ± 0.035
500	70.4 ± 8.2	0.338 ± 0.024

CALCULATED STATISTICS:

Related to daily initial concentrations:
EC10 = 70 µg test item/L
EC20 = 270 µg test item/L
LOEC = 51 µg test item/L
NOEC = 9.8 µg test item/L
Related to mean measured concentrations:
EC10 = 6.3 µg test item/L
EC20 = 23 µg test item/L
LOEC = 3.6 µg test item/L

NOEC = 1.6 µg test item/L

Test substance:
C14 Fatty alcohol (1-Tetradecanol)
CAS No. 112-72-1
Sample received from Laboratory Dr. Ehrenstorfer-Schafers, Augsburg, Germany.
Lot No: 30527
Purity: 99.5 % ± 0.5 %

Test substance: C10 Fatty alcohol (1-Decanol)
CAS No. 112-30-1
Sample received from Laboratory Dr. Ehrenstorfer-Schafers, Augsburg, Germany.
Lot No: 21011
Purity: 99.5 % ± 0.5 %

Reliability: (1) valid without restriction
Guideline study conducted in accordance with GLP.

Flag: Critical study for SIDS endpoint

Reference: Schafers, C. (2005). Daphnia magna, reproduction test in closed vessels following OECD 211. C12 fatty alcohol. GLP code: SDA-001/4-21. Fraunhofer Institute for Molecular Biology and Applied Ecology (IME) 57377 Schmallenberg, Germany.

04-NOV-2005 (62)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Species: Daphnia magna (Crustacea)

Endpoint: other: Survival, growth and reproduction rate

Exposure period: 21 day(s)

Method: other: read-across based on grouping of substances (category approach)

Year: 2005

GLP: no

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Method: Measured data of an acceptable quality are available for 21-day reproduction studies with Daphnia magna for the single carbon chain length alcohols 1-octanol (111-87-5), 1-decanol (112-30-1), 1-dodecanol (112-53-8; supporting), 1-tetradecanol (112-72-1) and 1-pentadecanol (629-76-5). The studies are described in the relevant dossiers and in Annex X to the SIAR. The data were obtained generally in accordance with standard test guideline OECD 211. No measured data are available for mixtures of different carbon chain length alcohols.

The data suggest that for substances of chain length greater than C15, no chronic effects would be expected.

Result: No chronic effects would be expected for this substance.

Reliability: (2) valid with restrictions
Value estimated based on findings for similar substances (other Category members) in reliable studies.

Flag: Critical study for SIDS endpoint

Reference: Annex X (2005). Chronic Toxicity of Long Chain Alcohols to Daphnia magna; Annex X to the Long Chain Aliphatic Alcohols SIAR.

21-DEC-2005 (7)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Species: Daphnia magna (Crustacea)

Endpoint: other: reproduction rate and mortality

Exposure period: 21 day(s)

Unit: mg/l **Analytical monitoring:** yes

NOEC: = .98

LOEC: = 2.94

Method: other: comparable to OECD Guide-line 202, part 2 "Daphnia sp., Reproduction test"

Year: 1992

GLP: yes

Test substance: other TS: Octadecanol (112-92-5)

Method: Chronic toxicity testing in Daphnia magna according to UBA toxicity testing protocol 'Prolonged toxicity test with Daphnia Magna', 01.02.1984; determination of the NOEC for reproduction rate, mortality and the moment of the first appearance of descendants.

Remark: Data refer to both mortality of parents and number of offspring/parent. The test substance was added directly, without the use of solvents. Note that the NOEC is approximately 100 times the solubility of octadecanol in water. Test conducted in 1992.

Result: RESULTS:

Concentration (mg/L)	0	1	3	10	30	100
First day of offspring	9-12	9-12	9-12	9-12	9-12	9-12
Survival rate of adults (%)	90	90	70	70	60	55

Average number of young 106 101 81 56 56 45
animal per adult
Standard deviation 3.5 21.5 17.6 20.7 8.6
12.1

Significant (p<0.05) -- no yes yes yes
yes

NOEC = 0.98 mg/L
LOEC = 2.94 mg/L

CONTROL SUBSTANCE:
No use of control substance reported.

Source: Guhl 1992.

Test condition: TEST ORGANISMS
Strain: Daphnia magna
Supplier: Own breeding, strain is identical with that of BGA
Age: not reported
Feeding: 1 ml algae (1-3 * 10E6 cells/ml) and 1 ml activated
sludge
Feeding during test: Monday/Wednesday/Friday
Control group: 1 group (4 replicates)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none (test substance was weighed directly
into test vessels)
Concentration of vehicle/solvent: not applicable
DILUTION WATER
Source: Aerated tap water
Aeration: not reported
Alkalinity: not reported
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: 1, 3, 10, 30 and 100 mg/l
Renewal of test solution: Monday/Wednesday/Friday
Exposure vessel type: 500 ml Erlenmeyer flasks
Number of replicates: 4
Animals per replicate: 5
Test temperature: 19-23 C
Dissolved oxygen: not reported
pH mean: 8.3-8.5
Adjustment of pH: not reported
Intensity of irradiation: Radium 60W
Photoperiod: 16 hours light, 8 hours dark
TEST PARAMETER: reproduction rate and mortality
MONITORING OF TEST SUBSTANCE CONCENTRATION: 0, 48 and 120

hours. Mean measured (DOC) concentrations in the 10 mg/l group were 0.7, 1.15 and 1.95 mg/l at 0, 48 and 120 hours, respectively. Similar measured concentrations were obtained in the 30 and 100 mg/l groups.

Reliability: (2) valid with restrictions
Best study although not a SIDS endpoint.

Reference: Guhl, Dr. 1992. Octadecanol (Lorol C18-98): Bestimmung der chronischen Daphnientoxizitat im verlangerten Daphnientest, 21 Tage. Henkel KGaA Report No. RE 920096.

30-OCT-2003 (4)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Species: Daphnia magna (Crustacea)
Endpoint: other: Survival, growth and reproduction rate
Exposure period: 21 day(s)

Method: other: read-across based on grouping of substances (category approach)
Year: 2005
GLP: no
Test substance: >= 90% 1-eicosanol (629-96-9)

Method: Measured data of an acceptable quality are available for 21-day reproduction studies with Daphnia magna for the single carbon chain length alcohols 1-octanol (111-87-5), 1-decanol (112-30-1), 1-dodecanol (112-53-8; supporting), 1-tetradecanol (112-72-1) and 1-pentadecanol (629-76-5). The studies are described in the relevant dossiers and in Annex X to the SIAR. The data were obtained generally in accordance with standard test guideline OECD 211. No measured data are available for mixtures of different carbon chain length alcohols.

The data suggest that for substances of chain length greater than C15, no chronic effects would be expected.

Result: No chronic effects would be expected for this substance.

Reliability: (2) valid with restrictions
Value estimated based on findings for similar substances (other Category members) in reliable studies.

Flag: Critical study for SIDS endpoint

Reference: Annex X (2005). Chronic Toxicity of Long Chain Alcohols to Daphnia magna; Annex X to the Long Chain Aliphatic Alcohols SIAR.

21-DEC-2005 (6)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Species: Daphnia magna (Crustacea)
Endpoint: other: Survival, growth and reproduction rate
Exposure period: 21 day(s)

Method: other: read-across based on grouping of substances (category approach)
Year: 2005
GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Method: Measured data of an acceptable quality are available for 21-day reproduction studies with Daphnia magna for the single carbon chain length alcohols 1-octanol (111-87-5), 1-decanol (112-30-1), 1-dodecanol (112-53-8; supporting), 1-tetradecanol (112-72-1) and 1-pentadecanol (629-76-5). The studies are described in the relevant dossiers and in Annex X to the SIAR. The data were obtained generally in accordance with standard test guideline OECD 211. No measured data are available for mixtures of different carbon chain length alcohols.

The data suggest that for substances of chain length greater than C15, no chronic effects would be expected.
Result: No chronic effects would be expected for this substance.
Reliability: (2) valid with restrictions
Value estimated based on findings for similar substances (other Category members) in reliable studies.
Flag: Critical study for SIDS endpoint
Reference: Annex X (2005). Chronic Toxicity of Long Chain Alcohols to Daphnia magna; Annex X to the Long Chain Aliphatic Alcohols SIAR.
21-DEC-2005 (6)

<u>1-Tetracosanol (506-51-4) for 1-Tetracosanol Aluminum Salt (67905-29-7)</u>

Unit: mg/l
Analytical monitoring: no
LC50: = 8.41×10^{-6} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-tetracosanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.

Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, 2006.
05-APR-2007

1-Hexacosanol (506-52-5) for 1-Hexacosanol Aluminum Salt (67905-28-6)

Unit: mg/l
Analytical monitoring: no
LC50: = 1.72×10^{-6} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-hexacosanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, 2006.
05-APR-2007

1-Octacosanol (557-61-9) for 1-Octacosanol Aluminum Salt (67905-27-5)

Unit: mg/l
Analytical monitoring: no
LC50: = 3.72×10^{-7} calculated

Method: other
Year: 2006
GLP: no
Test substance: 1-octacosanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, 2006.
05-APR-2007

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Unit: mg/l
Analytical monitoring: no
LC50: = 7.82×10^{-8} calculated

Method: other
Year: 2006

GLP: no
Test substance: 1-triacontanol

Method: ECOSAR v0.99, USEPA (2006).
Result: Predicted to be non-toxic at the limit of solubility.
Reliability: (2) valid with restrictions
Reference: ECOSAR v0.99. US EPA, 2006.
05-APR-2007

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5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LD50
Value	= 9.8 - 11.6 ml/kg bw
Species	Mouse
Strain	NMRI
Sex	male/female
Number of animals	5
Vehicle	physiol. saline
Doses	3 doses lying between LD16 and LD84
Method	other
Year	1976
GLP	no data
Test substance	other TS: Analytical grade ethanol (64-17-5)
Remark	Method: Ethanol administered to SPF NMRI mice (5 per sex per group) by gavage, diluted as necessary with physiological saline (0.9% NaCI). Volume administered was 20 ml/kg, or where necessary, 30 ml/kg. Quantities of solvent were varied so that at least three mortality values between 16 and 84% were obtained. All deaths occurred within 24 h. No signs or necropsy findings described. LD50 calculated by pro bit analysis and is for both sexes combined. Time of death: All occurred within 24 hr. Individual times not given. Description, severity, time of onset and duration of clinical signs at each dose level: Not described. Necropsy findings: Not done. Potential target organs: Not discussed. Sex comparison: Not given; LD50 is for both sexes combined.
Result	Values cited are 95% confidence limits. Values cited are 95% confidence limits. Average LD50=10.5ml/kg, which is equivalent to 8300mg/kg. LD50's for Lv. and Lp. routes also determined:- Lv. 2.8 Lp.4.0
Test condition	Age of animals: not given. Animals (5 of each sex) were housed in polycarbonate cages in air-conditioned rooms at a temperature of 22 deg.
Test substance	

C and relative humidity of 55%.
Food (Ssniff Standard diet R from Intermast GmbH, Bockum-Hovel) and water were available ad lib.
Doses: Not stated. At least 3 doses between LD16 and LD84 were used.

Doses per time period: One.
Volume administered or concentration: 20 ml/kg total volume.
Post dose observation period: 7 days.
Exposure duration: Not applicable.
Test substance was analytical grade.

Reliability (2) valid with restrictions
Flag Critical study for SIDS endpoint
Reference Bartsch, W. et at (1976) Acute toxicity of various solvents in the mouse and rat. Arzneim. Forsch. 26, 1581-1583.
12.11.2004 (151)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type LC50
Value = 15010 mg/kg bw
Species Rat
Strain
Sex Female
Number of animals 8
Vehicle other: gavaged after
Doses 5% gum acacia 16,17,18,19,20,21 ml/kg
Method other
Year 1992
GLP no data
Test substance ethanol (64-17-5)

Remark 19 ml/kg converts to 15.01 g/kg bw.
Method used female rats only, 8 per dose and 7 dose levels.

Ethanol gavage was preceeded by gum acacia gavage, intended to reduce local irritation in stomach.

Post dose observation period was 24 h.

Potential target organs, male-female comparison, necropsy findings not reported.
Time of death: Individual times not given.
Description, severity, time of onset and duration of clinical signs at each dose level: Inebriation to gait disturbance, dose-related decrease inresponse to painful stimuli, respiratory depression and

	coma. Necropsy findings: Diffuse congestion of the gastric mucosa without gross haemorrhage or ulceration. Potential target organs: Not discussed. Sex comparison: Not applicable.
Result	Clinical observations ranged from inebriation to gait disturbance and dose-related decrease in response to painful stimuli, repiratory depression and coma. Deaths were due to cardiorespiratory failure.
Test condition	Age of animals: Adults, 180 g. Animals were housed at a temperature of 22-26 degC with 12 hr light-12 hr dark cycle. Food and water were available ad lib. Doses: 16,17, 18,20,21 and 22 ml/kg. Doses per time period: One. Volume administered or concentration: See above. Post dose observation period: 24 hrs. Exposure duration: Not applicable.
Test substance	Test substance was 99.8% ethanol and 0.1 % methanol.
Reliability	(2) valid with restrictions Critical study for SI DS endpoint
Reference	Youssef, A., Madkour, K., Cox, C., Weiss, B. (1992) Comparative lethality of methanol, ethanol and mixtures in female rats. J. Appl. Toxicol. 12(3):193-197.
12.11.2004	(152)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	LD50
Value	7000 - 11000 mg/kg bw
Species	Rat
Strain	Wistar
Sex	Male
Number of animals	10
Vehicle	no data
Doses	six to 8 dose levels
Method	other
Year	1970
GLP	no data
Test substance	ethanol (64-17-5)
Method	Rats were about 100 days old in one experiment, 10-12 months old in another. Six to eight dose levels with a dose interval of 1.1 used. Ethanol given as a 40% w/v solution.
Remark	Results range of values for old rats to young rats. Time of death: All deaths occurred within 24 hr. Individual times not given.

	Description, severity, time of onset and duration of clinical signs at each dose level: Not described. Necropsy findings: Not conducted. Potential target organs: Cause of death was respiratory failure. Sex comparison: Not applicable.
Test condition	Age of animals: About 100 days or 10-12 mth. Food and water were available ad lib. Doses: 6-8 dose levels, not described. Doses per time period: One. Volume administered or concentration: As a 40% w/v solution. Post dose observation period: 24 hrs. Exposure duration: Not applicable.
Conclusion	Old rats were considerably more sensitive than young rats.
Reliability	(2) valid with restrictions Critical study for SIDS endpoint
Reference	Wiberg, G., Trenholm, H., Coldwell, B. (1970). Increased ethanol toxicity in old rats: changes in LD50, in vivo and in vitro metabolism, and liver alcohol dehydrogenase activity. Toxicol. Appl. Pharmacol. 16: 718-727.
12.11.2004	(153)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	LD50
Value	= 9.8 - 11.6 ml/kg bw
Species	Mouse
Strain	NMRI
Sex	male/female
Number of animals	5
Vehicle	physiol. saline
Doses	3 doses lying between LD16 and LD84
Method	other
Year	1976
GLP	no data
Test substance	other TS: Analytical grade ethanol (64-17-5)
Remark	Method: Ethanol administered to SPF NMRI mice (5 per sex per group) by gavage, diluted as necessary with physiological saline (0.9% NaCI). Volume administered was 20 mllkg, or where necessary, 30 ml/kg. Quantities of solvent were varied so that at least three mortality values between 16 and 84% were obtained. All deaths occurred within 24 h. No signs or necropsy findings described.

	LD50 calculated by pro bit analysis and is for both sexes combined. Time of death: All occurred within 24 hr. Individual times not given. Description, severity, time of onset and duration of clinical signs at each dose level: Not described. Necropsy findings: Not done. Potential target organs: Not discussed. Sex comparison: Not given; LD50 is for both sexes combined.
Result	Values cited are 95% confidence limits. Values cited are 95% confidence limits. Average LD50=10.5ml/kg, which is equivalent to 8300mg/kg. LD50's for Lv. and Lp. routes also determined:- Lv. 2.8 Lp.4.0
Test condition	Age of animals: not given. Animals (5 of each sex) were housed in polycarbonate cages in air-conditioned rooms at a temperature of 22 deg.
Test substance	C and relative humidity of 55%. Food (Ssniff Standard diet R from Intermast GmbH, Bockum-Hovel) and water were available ad lib. Doses: Not stated. At least 3 doses between LD16 and LD84 were used. Doses per time period: One. Volume administered or concentration: 20 mllkg total volume. Post dose observation period: 7 days. Exposure duration: Not applicable. Test substance was analytical grade.
Reliability	(2) valid with restrictions
Flag	Critical study for SIDS endpoint
Reference	Bartsch, W. et al. (1976) Acute toxicity of various solvents in the mouse and rat. Arzneim. Forsch. 26, 1581-1583.
12.11.2004	(151)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	LD50
Value	= 14.6 ml/kg bw
Species	Rat
Strain	Sprague-Dawley
Sex	Male
Number of animals	6
Vehicle	other: none
Doses	
Method	other
Year	1971

GLP	no data
Test substance	other TS: analytical grade ethanol (64-17-5)
Method	Age at start of treatment: Older rats (300-470 g). Dosing by straight needle in undiluted form in non-fasted animals. LD50 determined by method of Litchfield and Wilcoxon.
Result	95% confidence limits of result: 12800-16700mg/kg.
Reliability	(4) not assignable Very little method descrption was given.
Reference	Kimura, E.T., Ebert. D.M., Dodge, P.W. (1971). Acute toxicity limits of solvent residue for sixteen organic solvents. Toxicol Appl Pharmacol 19: 699-704.
12.11.2004	(154)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LD50
Value	7800 mg/kg bw
Species	Rat
Strain	Sprague-Dawley
Sex	male/female
Number of animals	
Vehicle	other: none
Doses	
Method	other
Year	1971
GLP	no data
Test substance	other TS: analytical grade ethanol (64-17-5)
Method	Age at start of treatment: 14 day old rats (16-50 g). Dosing by straight needle in undiluted form in non-fasted animals. LD50 determined by method of Litchfield and Wilcoxon. Number of animals: 6-12 95% confidence limits of result: 6300-9700mg/kg.
Reliability	(4) not assignable Very little detail provided of test method
Reference	Kimura, E.T., Ebert. D.M., Dodge, P.W. (1971). Acute toxicity limits of solvent residue for sixteen organic solvents. Toxicol Appl Pharmacol 19: 699-704.
12.11.2004	(155)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LD50
Value	11170 -16710 mg/kg bw
Species	Rat
Strain	

Sex	
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)

Method	
Reliability	(4) not assignable
Reference	Smyth, H.F. Jr. (1941) J. Ind. Hyg. Toxicol. 23, 253, cited in Patty (1982) loc. cit.
12.11.2004	(156)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LD50
Value	= 7060 mg/kg bw
Species	Rat
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)

Reliability	(4) not assignable
Reference	Anon. (1935) Am. J. Clin. Pathol. 5, 466 cited in RTECS (1992) loc. cit.
12.11.2004	(157)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LD50
Value	ca. 11850 mg/kg bw
Species	Rat
Method	other
Year	
GLP	No
Test substance	ethanol (64-17-5)

Remark	BASF Test. LD50 value was between 11850 and 12640mg/kg. test substance was ethanol at 90%.70% 50% and 30%.
Reliability	(4) not assignable
Reference	BASF AG Toxicology Department Unpublished report 26-01-1959.
12.11.2004	(158)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LD50
Value	= 9500 mg/kg bw
Species	Mouse
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Test Substance	Test substance was 95% ethanol.
Reliability	(4) not assignable
Reference	Latven, J. (1933) J. Pharm. Exp. Ther. 65,89. cited in Spector, W.S. (editor), 1965. Handbook of Toxicology. Vol. 1. Acute toxicities of solids, liquids and gases to laboratory animals. Saunders, Philadelphia and London.
12.11.2004	(159)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	LD50
Value	3450 mg/kg bw
Species	Mouse
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Method not specified.
Reliability	(4) not assignable
Reference	Anon. (1967) Gig. Sanit 32,31. cited in RTECS (1992) loc. cit.
12.11.2004	(160)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	LD50
Value	> 790 mg/kg bw
Species	Mouse
Method	other
Year	1972
GLP	No
Test substance	ethanol (64-17-5)
Remark	Converted from 10ml/kg.
Reliability	(4) not assignable
Reference	Bayer EU Existing Chemicals Programme HEDSETAG data

	February 15, 1972.
12.11.2004	(161)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LD50
Value	5060 - 7850 mg/kg bw
Species	Rabbit
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Value = 6300 mg/kg body weight
Reliability	(4) not assignable
Reference	Smyth, unpublished data, Mellon Inst. cited in Spector (1956) loc. cit.
12.11.2004	(162)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LDLo
Value	= 7000 mg/kg bw
Species	Rabbit
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Method not specified.
Reliability	(4) not assignable
Reference	Takeda, I. (1972) Nichidai Igaku Zasshi 31, 518 cited in Patty (1982) loc. cit.
12.11.2004	(163)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Other
Value	= 9900 mg/kg bw
Species	Rabbit
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Although the value was reported as an LD50 value, in a later

	publication (Munch J.C.1972. Ind. med. Surg.41, 31) it is said to be the minimum lethal dose.
Reliability	(4) not assignable
Reference	Munch, J.C. & Schwartze, E.W. (1925) J. Lab. Clin. Med. 10, 985. cited in Patty (1982) loc. cit.
12.11.2004	(164)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LDLO
Value	= 6000 mg/kg bw
Species	Cat
Method	other
Year	1936
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Method not specified.
Reliability	(4) not assignable
Reference	Anon. (1936) J. Pharmac. Exp. Ther. 56, 117 cited in RTECS (1992) loc. cit.
12.11.2004	(165)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Other
Value	5500 - 6500 mg/kg bw
Species	Dog
Method	other
Year	1875
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Time of death reported to be "12 to 14 hours". Value is reported as the lethal dose.
Reliability	(4) not assignable
Reference	DuJardin-Beaumetz, C. (1875) Rend. Acad. Sc. 81, 192. cited in Spector (1956) loc. cit.
12.11.2004	(166)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Other
Value	
Species	Dog
GLP	no data

Test substance	ethanol (64-17-5)
Remark	30% aqueous ethanol. Dogs were dosed by gavage with 4ml/kg (ca. 3160mg/kg) or 8mls/kg (ca. 6320mg/kg) of 33% aqueous ethanol solution. (4ml/kg dosed within 1 hour, 8 ml/kg dosed within 2 hours). Liver function was tested by use of Bromosulphothalein (BSP) tests. The 8ml/kg ethanol dosed group gave an mean increased SSP retention time of ca. 10% that of the 4ml/kg group.
Reliability	(4) not assignable
Reference	BASF AG Toxicology Department Unpublished research 26-01-1959.
12.11.2004	(167)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	LD50
Value	= 5560 mg/kg bw
Species	guinea pig
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	
Reliability	(4) not assignable
Reference	Smyth, H.F. Jr. (1941) J.lnd. Hyg. Toxicol. 23, 259 cited in RTECS (1992) loc. cit.
12.11.2004	(168)

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Test substance:	1-Butanol, Union Carbide sample procured 12/20/48 from Fellowship 155.
Method:	Method/guideline followed: Internal Union Carbide method (gavage). Thompson's method of calculating median-effective dose.
Test type:	Acute oral by gavage
GLP:	No
Year performed:	12/48 - 1/49
Species/strain:	Rat, albino Sherman
Sex:	Female, 5-6 weeks old, 90-120 grams.
Number of animals:	10
sex/dose:	females/dose

Vehicle: 20% dispersion of n-butanol in 1 % Tergitol 7.
Route of admin.: orally in liquid.
Results LD50 = 4.36 (3.98 to 4.78) g/kg

Number of deaths at each dose level: 10/10 at 6.3 g/kg.
8/10 at 5.0 g/kg.
3/10 at 3.98 g/kg. 0110 at 3.16 g/kg.

Comments: After 6.3 g/kg dose, six rats died on day 0 and four rats died on day 1. After 5.0 g/kg dose, four rats died on day 0 and four rats died on day 1. After 3.98 g/kg dose, one rat died on day 0, one rat died on day 1, and one rat died on day 3. After 3.16 g/kg dose, all ten rats survived for the total observation period of 14 days.

11,9, and 1 deaths occurred on days 0, 1, or 3, respectively. Narcosis and prostration preceded death. It could not be determined from the study report whether narcosis was observed at the . lowest dose tested. T he higher doses produced hemorrhage of the stomach and intestinal irritation. Livers were congested and kidneys pale.

Data quality: Reliability: Key study. Klimisch quality 2.
References: Union Carbide Corp. Bushy Run Research Center, Project Report No.14-73. Export, P A. 1951.

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Test substance: 1-Butanol, Union Carbide undiluted sample.
Method: Method/guideline followed: Internal Union Carbide method (intubation). The moving average method of calculating median-effective dose was used based upon a 14-day observation period.
Test type: Acute oral by gavage.
GLP: No

Year performed: Not specified.
Species/strain: Rat, Harlan Wistar.
Sex: Female, 60 days old, 180-260 grams.
Number of animals:
sex/dose: Not specified.
Vehicle: None
Route of admin. : Orally as neat (undiluted) liquid.
Results: LD50 2.83 ml/kg 2.290 g/kg = 2290 mg/kg
Number of deaths at each dose level: Not specified.
Comments: Dosage levels differed by a factor of 2 in a geometric series.
Data quality: Reliability: Key study. Klimisch quality 2.
References: Union Carbide Corp. Bushy Run Research Center, Project Report

No. 29-126. Export, PA. 1966.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance:	1-Butanol, Union Carbide undiluted sample.
Method:	Method/guideline followed: Internal Union Carbide method (intubation). The moving average method of calculating median-effective dose was used based upon a 14-day observation period.
Test type:	Acute oral by gavage.
GLP:	No
Year performed:	Not specified.
Species/strain:	Rat, Harlan Wistar.
Sex:	Female, 60 days old, 180-260 grams.
Number of animals:	
sex/dose:	Not specified.
Vehicle:	None
Route of admin. :	Orally as neat (undiluted) liquid.
Results:	LD50 2.83 ml/kg 2.290 g/kg = 2290 mg/kg Number of deaths at each dose level: Not specified.
Comments:	Dosage levels differed by a factor of 2 in a geometric series.
Data quality:	Reliability: Key study. Klimisch quality 2.
References:	Union Carbide Corp. Bushy Run Research Center, Project Report No. 29-126. Export, PA. 1966.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance:	Identity: 1-Butanol.
Method:	Method/guideline followed: FDA method. LDso's were computed by the method of Litchfield & Wilcoxon.
Test type:	Acute oral toxicity by gavage.
GLP:	No
Year performed:	Not specified.
Species/strain:	Rat, adult Osborne-Mendel.
Sex:	Male and female, evenly divided.
Number of animals:	
sex/dose:	5/sex/dose.
Vehicle:	
Route of admin. :	Orally by gavage as a neat (undiluted) liquid. Animals were fasted approximately 18 hours prior to administration.
Results:	LD50 = 2.51 (2.22 to 2.84) g/kg
Comments:	Observation period was 14 days postdosing. Symptoms included depression and coma. Mortality occurred between 4 and 18 hours

postdosing.

Data quality: Reliability: Klimisch quality 2.

References: Jenner, P.M., Hagan, E.C., Taylor, J.M., Cook, E.L., and Fitzhugh,O.G. 1964. Food flavourings and compounds of related structure. I. Acute oral toxicity. Fd. Cosmet. Toxieol. 2: 327-343.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species/strain: Rat, male and female (unspecified strain)
Test method: single dose, stomach tube
GLP: No

Test results: LD50 2.02 g/kg, male *
LD50 = 0.79 g/kg, female *

Comments: The 95% confidence intervals overlapped, indicating that the LD50's were not significantly different for male or female.

Reference: Purchase L.H.F. Studies in Kaffir Corn Malting and Brewing. XXII. The Acute Toxicity of Some Fusel Oils Found in Bantu Beer. So. Afr. Med. Jor. 43 (25): 795-798. 1969.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-butanol
Test species/strain: Mouse (unspecified strain)
Test method: Not Stated
GLP: No

Test results: LD50 2.68 g/kg

Reference: Rumyanstev A.P., Lobanova I.Y A., Tiunova L.V. and Chernikova V.V. Toxicology of Butyl Alcohol Khim. Prom.-st. Ser. Toksikol. San it. Khim. Plastmass. 2:24-26. 1979.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species/strain: Rabbit (unspecified strain)
Test method: single dose, stomach tube
GLP: No

Test results: LD50 = 3.5 g/kg 24-Hr.
*ND50 = 0.8 g/kg

Comments: * ND50 is the quantity that caused narcosis in half the rabbits.

Reference: Munch J.C. Aliphatic Alcohols and Alkyl Esters: Narcotic and

Lethal Potencies to Tadpoles and to Rabbits. Ind. Med. Surg. 41(4):31-33.1972.

Munch J.C. and Schwarze E.W. Narcotic and Toxic Potency of Aliphatic Alcohols upon Rabbits. Jar. Lab. Clin. Med. 10: 985-996. 1925.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species/strain: Golden hamster
Test method: Not Stated
GLP: No
Test results: * LD50 1.2 g/kg
Comments: * 95% confidence limits 0.6-2.3 g/kg
Reference: Dubina O.N. and Maksimov G.G. Testing the use of Golden Hamsters in Toxicological Research, Gig. Tr. Ohkhr. Zdorov'ya Rab. Neft. Neftekhim. Prom-sti. 9: 100-103. 1976.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species/strain: Dog
Test method: Not Stated
GLP: No

Test results: LD50 2.2 ml/kg = 1.782 g/kg = 1782 mg/kg
Comments: LD50 = The minimum fatal dose.
Reference: Von Oettingen W.F. The aliphatic alcohols, their toxicity and potential dangers in relation to their chemical constitution and their fate in metabolism. U.S. Public Health Service., Public Health Bulletin., No. 281. D.S. Government Printing Office., Washington D.C. 1943.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LD50
Species: rat
Strain: other: Holtzman albino
Sex: male/female
No. of Animals: 60
Vehicle: other: undiluted
Doses: 1.17, 1.65, 2.33, 3.28, 4.64 and 6.55 gm/kg
Value: = 3210 mg/kg bw

Method: other: not specified
Year: 1965

GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: MORTALITY:
- Time of death: All deaths occurred within 24 hours of dosing

- Number of deaths at each dose: 0/10, 1/10. 4/10. 4/10, 8/10, 8/10.

CLINICAL SIGNS: Animals at all dose levels exhibited weakness and ataxia. They became comatose and breathing was laboured while comatose. Animals which survived appeared normal within 24 hours other than top dose animals (6.55 g/kg) where the rats appeared unwell up to 48 hours after dosing. Weight gain amongst survivors was within normal limits.

NECROPSY FINDINGS: Necropsy of animals which died showed congestion of the lungs and adrenals in most animals. In some cases gastric congestion was also observed. There were no remarkable gross findings in animals sacrificed at the end of the observation period.

POTENTIAL TARGET ORGANS: No conclusion drawn.

SEX-SPECIFIC DIFFERENCES: None reported, mortality was presented as a combined value so no independent assessment can be made.

Source: Scientific Associates, Inc. 1965a
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS:
- Source: No data
- Weight at study initiation: 200 - 265 g
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION:
- Doses: 1.17, 1.65, 2.33, 3.28, 4.64 and 6.55 gm/kg
- Doses per time period: single
- Volume administered or concentration: Undiluted
- Post dose observation period: 14 days.

EXAMINATIONS: The animals were observed several times on the day of dosing and daily thereafter. Gross necropsies were performed on all survivors and any animals which died during the observation period. Body weights of survivors were recorded prior to sacrifice.

The LD50 was calculated using the method of Litchfield and Wilcoxon.

Test substance: Trade name Alfol 6

Conclusion: The rat oral LD50 value (M+F) for Alfol 6 was 3.21 g/kg confidence limits 2.35 to 4.39 g/kg. No specific target organ was identified.

Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
Well documented and conducted study.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3

Scientific Associates, Inc. 1965a. Acute oral toxicity (LD50) study in rats. Alfol 6.
15-JUL-2005 (29) (59)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LD50
Species: rat
Strain: other: COX-SD
Sex: male/female
No. of Animals: 50
Vehicle: other: undiluted
Doses: 2, 3.17, 5.02, 6.32 and 7.96 g/kg
Value: = 4420 mg/kg bw

Method: other: in house protocol
Year: 1977
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: MORTALITY:
- Time of death: All decendents died on the day of dosing.
- Number of deaths at each dose: 0/10; 0/5M 3/5F; 2/5M 3/5F; 3/5M, 4/5F; 10/10.

Rat oral LD504.42 g/kg (confidence limits 3.95 - 4.95).

CLINICAL SIGNS: At the lowest dose (2g/kg) 6 animals showed no signs of intoxication. The 4 remaining animals and all animals at the higher dose levels showed one or more of the following: Hypoactivity, diarrhoea, hypersalivation. hyper lacrymation, haematuria, maliase, ataxia, proneness, loss of righting reflex and sedation. All survivors returned to normal between

24 and 72 hours after dosing. With the exception of 1 male at the 6,32 g/kg level which showed a poor weight gain all other survivors gained weight within expected limits.

NECROPSY FINDINGS: Animals which died prematurely showed one or more of the following gross abnormalities: moderate to severe congestion of the kidneys, adrenals, lungs, liver, stomach and gastrolintestinal tract. There was thickening (translucent portion) and erosion of the gastric mucosa.

Animals necropsied at sacrifice showed in all proliferation of the gastric mucosa (translucent portion) up to 10-90% in some rats. Also observed in some rats adhesion of the stomach to major abdominal organs and/or the abdominal wall and pallor of the pancreas. One rat showed a whitish-green kidney medulla.

POTENTIAL TARGET ORGANS: Gastric mucosa.

SEX-SPECIFIC DIFFERENCES: Females appear more sensitive based on mortality data.

Source: Scientific Associates, Inc. 1977c
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rat (COX-SD)
- Source: Not reported.
- Age: Not reported
- Weight at study initiation: 198-254g
- Group size: 5M+5F/group fasted

- Controls: No

ADMINISTRATION: Oral gavage
- Doses: 2, 3.17, 5.02, 6.32 and 7.96 g/kg
- Doses per time period: single
- Volume administered or concentration: Undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs were recorded several times on the day of dosing and thereafter daily throughout the observation period. All premature decedents and survivors were subject to gross necropsy. All surviving animals were weighed prior to sacrifice. the LD50 was calculated using the method of Litchfield and Wilcoxon, 1949.

Test substance: Tradename Alfol 6

Conclusion: The rat oral LD50 for Alfol 6 was 4.42 g/kg. The gastric mucosa appears to be a target organ.

Reliability: (2) valid with restrictions

Comparable to guideline study with acceptable restirictions.
Well documented and well conducted study.
Flag: Critical study for SIDS endpoint
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3

Scientific Associates, Inc. 1977c. Acute oral toxicity (LD50) in rats; Acute dermal toxicity (LD50) in rabbits, Dermal irritation test in rabbits; Eye irritation test in rabbits; Inhalation toxicity tests in rats: ALFOL 6. S.A. Number 233619.
11-NOV-2004 (29) (62)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LD50
Species: mouse
Sex: male/female
Vehicle: other: undiluted
Doses: not reported
Value: = 4000 mg/kg bw

Method: other
Year: 1963
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Result: The mouse LD50 value for n-hexanol is 4 g/kg. Signs of intoxication were lack of coordination, respiratory distress, hyperactivity and convulsive twitching. Pathological examination of mice which died revealed hyperaemia of the internal organs and brain.
Source: Zaeva, 1963
Hayes Consultancy Service Bromley, Kent
Test condition: Groups of 6 mice received the test material undiluted at various dose levels (these ranged between 1 and 35 g/kg). The actual dose levels were not reported. The animals were observed for 14 days after dosing and the animals which died were subject to pathological examination. n-hexanol was tested as part of a comparative study with other alcohols.
Reliability: (4) not assignable
Original document in Russian (translation available), experimental detail limited but result considered valid.
Reference: Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

Zaeva, G.N. and Fedorova, V.I 1963 The toxicology of higher saturated monoatomic alcohols (n-hexyl, n-heptyl, n-octyl, n-nonyl and n-decyl). Toksikol. Novykh. Prom. Khim. Vesch. 5:51-55.
13-OCT-2004 (48) (85)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LD50
Species: rat
Strain: Sherman
Sex: male
Vehicle: other
Value: = 4590 mg/kg bw

Method: other: Smyth & Carpenter, 1944 & 1948
Year: 1951
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Result: Rat oral LD50 4590 mg/kg (confidence limits 4030-5940 mg/kg).
Source: Smyth et al, 1951
Test condition: Groups of 6 male rats received doses of the test material at 10 fold dose intervals, followed by 2 groups of 10 rats at intermediate doses as appropriate.
Reliability: (4) not assignable
Summary data on a number of substances, result valid but reporting limited.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

Smyth, H.F., Carpenter, C.P., and Weil, C.S. 1951. Range-finding toxicity data: List IV. A.M.A. Archives of Industrial Hygiene and Occupational Medicine 4: 119-122.
12-SEP-2004 (29) (48) (68)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LD50
Species: rat
Value: = 4870 mg/kg bw

Method: other

Year: 1967
Test substance: >95% 1-hexanol (111-27-3)

Remark: Value reported in Patty 2000, no experimental details given. This value referenced to Baer & Griepentrog, 1967 which is itself a secondary reference.
Reliability: (4) not assignable
Secondary reference, original in German, no experimental details available.
Reference: Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.
13-OCT-2004 (48)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LD50
Species: rat
Sex: no data
Value: = 3131 - 3344 mg/kg bw

Method: OECD Guide-line 401 "Acute Oral Toxicity"
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Remark: No further experimental details available. Company data reported original report unavailable.
Test substance: Tradename Nacol 6 RD
Reliability: (4) not assignable
Secondary reference
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3
13-OCT-2004 (29)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LD50
Species: mouse
Sex: no data
Value: = 1950 mg/kg bw

Method: other: no data
Year: 1966
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Reliability: (4) not assignable

Secondary reference
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3

RTECS, 2004.
12-SEP-2004 (29) (55)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Test substance: 1-hexanol (111-27-3)
Remark: Several other LD50 values are reported in IUCLID 2000 ascribed to either Henkel (1) or the Dangerous Properties of Industrial Materials Report for hexanol (2).

The values are all for rats and are as follows:

LD50 4870 mg/kg and 4000 mg/kg (1)
LD50 4100 mg/kg and 4900 mg/kg (2)

No experimental details are given.
Reliability: (4) not assignable
Secondary references.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3
12-SEP-2004 (29)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: LD50
Species: rat
Strain: other: Holtzman albino
Sex: male/female
No. of Animals: 60
Vehicle: other: undiluted
Doses: 4680, 6600, 9330, 13170, 18600, and 26280 mg/kg bw
Value: = 18240 mg/kg bw

Method: other: not specified
Year: 1965
GLP: no
Test substance: > 90% 1-octanol (111-87-5)

Result: MORTALITY:
- Time of death: All deaths occured within 24 hours of dsoing.
- Number of deaths at each dose: 0/10, 0/10, 1/10, 0/10, 5/10, 8/10

CLINICAL SIGNS: On the day of dosing, diarrhea, weakness, ataxia and malaise were observed in most of the animals at the four highest test levels. Animals which did not die overnight returned to normal within 6 days, most within 2 days.

NECROPSY FINDINGS: Most animals which died had pulmonary and adrenal congestion. Some also had slight congestion of the stomach. In the sacrificed animals, weight gains were in the normal limits and gross necropsy did not reveal any remarkable findings. At the highest dose level, bloody encrustations about the nares were evident.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None reported, mortality was presented as a combined value so no independent assessment can be made.

Source: Scientific Associates, Inc. 1965b
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS:
- Source: No data
- Weight at study initiation: data given but document illegible at this point.
- Group size 5M+5F
- Controls: no

ADMINISTRATION:
- Doses: 1.17, 1.65, 2.33, 3.28, 4.64 and 6.55 gm/kg
- Doses per time period: not reported
- Volume administered or concentration: Undiluted

- Post dose observation period: 14 days.

EXAMINATIONS: The animals were observed several times on the day of dosing and daily thereafter. Gross necropsies were performed on all survivors and any animals which died during the observation period. Body weights of survivors were recorded prior to sacrifice.

The LD50 was calculated using the method of Litchfield and Wilcoxon.

Test substance: Tradename Alfol 8.

Conclusion: The rat oral LD50 value (M+F) for Alfol 8 was 18.24 g/kg confidence limits 14.25 to 23.34 g/kg. No specific target organ was identified.

Reliability: (2) valid with restrictions
Well documented and conducted study with acceptable restrictions.
Flag: Critical study for SIDS endpoint
Reference: Scientific Associates, Inc. 1965b. Acute oral toxicity (LD50) study in rats. ALFOL 8.
16-JUL-2005 (100)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: LD50
Species: rat
Strain: Wistar
Sex: male/female
No. of Animals: 10
Vehicle: other: as an aqueous suspension
Doses: 5 g/kg single dose level
Value: > 5000 mg/kg bw

Method: other: OECD 401 (limit test)
Year: 1981
GLP: yes
Test substance: > 90% 1-octanol (111-87-5)

Result: MORTALITY: There were no deaths during the course of the study.

CLINICAL SIGNS: During the first 24 hours all test animals showed some decrease in actvity and piloerection. The animals showed a gain in body weight at all measurement points during the 14 day observation period.

NECROPSY FINDINGS: The were no abnormal findings.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: No.
Source: Henkel KGaA 1981a
Hayes Consultancy Service Bromley, Kent
Test condition: TEST ORGANISMS: Rat (Wistar)
- Source: Winkelmann, Hanover, Germany
- Weight at study initiation: mean body weight males, 137, females 127
- Group size: 5M+5F
- Controls: no

ADMINISTRATION: Gavage animals fasted
- Doses: 5 g/kg
- Doses per time period: single dose
- Volume administered or concentration: administered as a 25% aqueous suspension at a constant volume of 20 ml/kg.
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs were observed particularly during the first 24 hours after dosing. Body weights were recorded prior to dosing and at 24 hours, 1 week and 2 weeks after dosing. All survivors were subject to gross necropsy at the end of the observation period.

Test substance: Tradename Lorol 8

Conclusion: The rat oral LD50 for Lorol 8 was >5g/kg when applied as an aqueous suspension. Clinical signs of intoxication were confined to slight sedation and piloerection during the first 24 hours following dosing. There was no remarkable gross pathology at necrospy and no indication of specific target organ toxicity.

Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
Well documented and conducted study.

Flag: Critical study for SIDS endpoint

Reference: Henkel KGaA. 1981a. 1-Octanol: Evaluation of acute oral toxicity. Unpublished data, Report No. R 9500186.
Publication no. 936.

Iuclid 2000 European Commission - European Chemicals Bureau
Octan-1-ol Cas# 111-87-5
16-JUL-2005 (50) (62)

<u>1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)</u>

Type: LD50
Species: rat
Strain: other: no data
Sex: no data
Value: > 3200 mg/kg bw

Method: other
GLP: no
Test substance: other TS: 2-octanol

Remark: This value is reported in several secondary references as being the LD50 value for n-octanol. These sources are erroneous, the original report in Patty 1963 of an unpublished

reference by Fassett is clearly a value for 2-octanol. This value does not appear in Patty 2001.

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Octan-1-ol Cas# 111-87-5.

Opdyke, D.L.J. 1973 Monographs on fragrance raw materials. Fd. Cos. Tox. 11: 95-115.

RTECS, 2004.

14-SEP-2004 (62) (88) (93)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: LD50
Species: rat
Value: > 5000 mg/kg bw

Method: other: no data
Year: 1973
GLP: no
Test substance: > 90% 1-octanol (111-87-5)

Remark: Secondary report of unpublished data from Levenstein, 1972 report to RIFM.

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Octan-1-ol Cas# 111-87-5

Opdyke, D.L.J. 1973 Monographs on fragrance raw materials. Fd. Cos. Tox. 11:95-115.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

14-SEP-2004 (62) (88) (90)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: LD50
Species: rat
Value: = 20000 mg/kg bw

Year: 1984
Test substance: > 90% 1-octanol (111-87-5)

Remark: Unspecified changes in the brain, liver and urinary system, no indication of dose level.
Reliability: (4) not assignable
Secondary reference to Russian language original, unobtainable.
Reference: RTECS, 2004.
17-OCT-2004 (93)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: LD50
Species: mouse
Value: = 1790 mg/kg bw

Method: other
Test substance: > 90% 1-octanol (111-87-5)

Remark: Secondary report of an unobtainable Russian study reported by RTECS.
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau Octan-1-ol Cas# 111-87-5.

RTECS, 2004.
07-OCT-2004 (62) (93)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: LD50
Species: mouse
Value: = 15000 mg/kg bw

Year: 1984
Test substance: > 90% 1-octanol (111-87-5)

Remark: Unspecified changes in the brain, liver and urinary system, no indication of dose level.
Reliability: (4) not assignable
Secondary reference to Russian language original, unobtainable.
Reference: RTECS, 2004.
17-OCT-2004 (93)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: LD50
Species: rat
Strain: other: COX-SD
Sex: male/female
No. of Animals: 60
Vehicle: other: Undiluted
Doses: 7.96, 12.62, 15.89, 20.00, 31.70 and 39.91 gm/kg
Value: = 19500 mg/kg bw

Method: other: contract laboratory procedure
Year: 1977
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Result: MORTALITY:
- Time of death: between days 1 and 7.
- Number of deaths at each dose: 0/10, 2/10, 3/10, 7/10, 7/10, 10/10

CLINICAL SIGNS: Animals at each dose level displayed one or more of the following effects: hypoactivity, hypersalivation, diarrhea, malaise, unthriftness, hypersensitivity to touch, ventral alopecia (abdominal and perineal areas), generalized weakness, and emaciation. Twenty-five of the surviving animals returned to normal 2 to 10 days after dosage. Moderate to severe hypersensitivity to touch, emaciation and ventral alopecia persisted in the remaining six animals throughout the observation period. The three survivors at the 31.7 g/kg bw level experienced moderate to severe body weight loss.

NECROPSY FINDINGS: Twenty-one of the animals which succumbed showed one or more gross abnormalities: congestion of the kidneys, adrenals, liver, lungs, stomach and gastrointestinal tract, erosion of the mucosa of the translucent stomach, and linear and/or diffuse haemorrhages. Sacrificed animals revealed a proliferation of the mucosal tissues and depletion and visceral fatty tissue.

Gross necropsy of the animals sacrificed showed, in one, erosion, in twenty, proliferation of the mucosal tissues of the translucent stomach, and in three a depletion of the visceral fatty tissue. Necropsy findings in the remaining 11 animals did not reveal anything remarkable.

POTENTIAL TARGET ORGANS: Stomach, possible irritation of the mucosal lining.

SEX-SPECIFIC DIFFERENCES: None.

Source: Scientific Associates, Inc. 1977d
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: rats COX-SD
- Source: No data
- Weight at study initiation: 195 -274 g
- Controls: no
- Number/group: 5M+5F fasted

ADMINISTRATION:
- Doses: 7.96, 12.62, 15.89, 20.00, 31.70 and 39.91 gm/kg
- Doses per time period: single dose
- Volume administered or concentration: Undiluted
- Post dose observation period: 14 days.

EXAMINATIONS: The animals were observed several times on the day of dosing and daily thereafter. Gross necropsies were performed on all survivors and any animals which died during the observation period. Body weights of survivors were recorded prior to sacrifice.

The LD50 was calculated using the method of Litchfield and Wilcoxon.

Test substance: Tradename Alfol 10

Conclusion: Rat oral LD50 of Alfol 10 is 19.5 g/kg (confidence limits (15.72-24.18), possible target organ, stomach mucosa.

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: Scientific Associates, Inc. 1977d. Acute oral toxicity (LD50) in rats. ALFOL 10 alcohol.

05-AUG-2005 (81)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Type: LD50
Species: rat
Strain: other: Holzman albiino
Sex: male/female
No. of Animals: 60
Vehicle: other: undiluted
Doses: 4.7, 6.63, 9.37, 13.24, 18.69, and 26.41 g/kg b.w.

Value: > 26410 mg/kg bw

Method: other: contract laboratory procedure
Year: 1965
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Result: MORTALITY: No animals died.

CLINICAL SIGNS: No signs of toxicity or pharmacological effects were observed in any of the animals on the day of dosing. Diuresis lasted for less than 72-hours after dosage at the three lowest test levels. Diuresis, weakness, malaise, and bloody nasal discharge were evident at the three highest doses for less than a week. Posterior ventral hair loss was noted at the three highest levels after 6-days. The sacrificed animals showed normal weight gains with one exception. One animal at the highest dose level showed a loss of 5 grams.

NECROPSY FINDINGS: Gross necropsy of the sacrificed animals showed no abnormalities of the viscera. Loss of hair of the posterior ventral surface of the body was evident in all animals at the three highest levels.

POTENTIAL TARGET ORGANS: No obvious target organs.

SEX-SPECIFIC DIFFERENCES: Combined observations were reported so no conclusion could be drawn.

Source: Scientific Associates, Inc. 1965c
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: rat
- Source: no data
- Weight at study initiation: 200-265 g
- Group size:5M+5F
- Controls: no

ADMINISTRATION:
- Doses: 4.7, 6.63, 9.37, 13.24, 18.69, and 26.41 g/kg b.w.
- Doses per time period: single
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: The animals were observed for clinical signs at regular intervals on the day of dosing and dialy thereafter. Following the 14 day observation perod all surviving animals were weighed, sacrificed and gross necropsies carried out. The

LD50 was calculated by the Litchfield and Wilcoxon method.
Test substance: Tradename Alfol 10
Conclusion: Rat oral LD50 for Alfol 10 is >26.41 g/kg.
Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
Flag: Critical study for SIDS endpoint
Reference: Scientific Associates, Inc. 1965c. Acute oral toxicity (LD50) study in rats. ALFOL 10.
05-AUG-2005 (78)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: LD50
Species: rat
Strain: Wistar
Sex: male
No. of Animals: 10
Vehicle: other: olive oil
Doses: 5 g/kg
Value: > 5000 mg/kg bw

Method: other
Year: 1979
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Result: MORTALITY: There were no deaths

CLINICAL SIGNS: There were no signs of toxicity.

POTENTIAL TARGET ORGANS: No conclusion could be drawn as there were no signs of toxicity and no pathological examination.

SEX-SPECIFIC DIFFERENCES: Males only tested.
Source: Potokar, 1979
Hayes Consultancy Service Bromley, Kent
Test condition: TEST ORGANISMS:
- Source: No data
- Age: adult
- Weight at study initiation: mean weight 170 g
- Controls: No

ADMINISTRATION:
- Doses: 5 g/kg
- Doses per time period: single dose

- Volume administered or concentration: 1ml/100g in olive oil.
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs and mortality.

Test substance: Tradename Lorol C10

Conclusion: The rat oral LD50 for Lorol C10 was >5 g/kg.

Also referred to in Iuclid 2000.

Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 ECB Decanol.

Potokar, 1979. Lorol 810 und Lorol C 10, Toxikologische Untersuchungen. No. 281. 27 November 1979.

25-NOV-2004 (53) (71)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Type: LD50
Species: rat
Strain: Wistar
Sex: male
No. of Animals: 10
Vehicle: other: undiluted
Doses: 5000 mg/kg
Value: > 5000 mg/kg bw

Method: other: The rats were administered the test substance by gavage in a limit test and observed for a 14-day period.
Year: 1979
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Result: No adverse effects were observed during the observation period. The LD50 for male rats is >5000 mg/kg bw.

Source: Henkel KGaA 1979
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rat
- Source: no data
- Weight at study initiation: no data
- Group size: 10M fasted
- Controls: no

ADMINISTRATION:
- Doses: 5000 mg/kg

- Doses per time period: single
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: observations of clinical signs and mortality.

Summary data only provided.

Reliability: (4) not assignable
Summary sheet only available, however would expect this to be a reasonable study as other Henkel reports are generally RL1 or 2.

Reference: Henkel KGaA. 1979. 1-Decanol: Evaluation of acute oral toxicity. Unpublished data, Report No. TBD 790158.

05-AUG-2005 (40)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Type: LD50
Species: mouse
Sex: male/female
No. of Animals: 6
Vehicle: other: undiluted
Doses: unspecified
Value: = 25000 mg/kg bw

Method: other
Year: 1963
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Result: The mouse LD50 value for 1-decanol is 25 g/kg. Signs of intoxication were lack of coordination, respiratory distress, hyperactivity and convulsive twitching. Pathological examination of mice which died revealed hyperaemia of the internal organs and brain.

Source: Zaeva, 1963
Hayes Consultancy Service Bromley, Kent

Test condition: Groups of 6 mice received the test material undiluted at various dose levels (these ranged between 1 and 35 g/kg), the actual dose levels were not reported. The animals were observed for 14 days after dosing and the animals which died were subject to pathological examination.

Reliability: (4) not assignable
Original document in Russian (translation available), experimental detail limited but result considered valid.

Reference: Zaeva, G.N. and Fedorova, V.I. 1963 The toxicology of higher

saturated monoatomic alcohols (n-hexyl, n-heptyl, n-octyl, n-nonyl and n-decyl). Toksikol. Novykh. Prom. Khim. Vesch. 5: 51-55.

05-AUG-2005 (106)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: LD50
Species: mouse
Strain: no data
Sex: no data
Value: = 6500 mg/kg bw

Test substance: other TS: decyl alcohol isomeric composition not specified

Remark: No other data available.
Reliability: (4) not assignable
Secondary reference. Original value reported in the Farm Chemicals Handbook 1991 which was not available for review and considered likely to be itself a secondary reference.
Reference: RTECS on line 2004 Decyl Alcohol.

05-AUG-2005 (74)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type	:	LD50
Species	:	rat
Strain	:	other: Holzman albino
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: undiluted
Value	:	> 26530 mg/kg bw
Method	:	other: standard in house procedure
Year	:	1965
GLP	:	no
Test substance	:	dodecanol (112-53-8)
Test substance	:	Tradename Alfol 12
Test condition	:	TEST ORGANISMS: rat - Source: not reported - Weight at study initiation: 210-265 g - Group size: 5M+5F - Controls: no ADMINISTRATION:

- Doses: 4.72, 6.66, 9.42, 13.30, 18.78 and 26.53 g/kg
- Doses per time period: single dose fasted overnight
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Observed for gross toxic effects several times on the day of dosing and daily thereafter for 14 days. Animals which died were necropsied. All survivors were weighed and necropsied at the end of the observation period.

Result : MORTALITY: There were no mortalities at any dose level.

CLINICAL SIGNS: No signs of toxicity or pharmacological effects were observed at any dose level on the day of dosing. Within 24 hours, diuresis was evident at all test levels. Weakness and bloody nasal discharge were exhibited by most of the animals at the top dose level (26.53 g/kg) at this time. These effects persisted for less than 72 hours. Hair loss of the posterior ventral surface of the body occurred in most of the animals at the two highest dosage levels at varying times throughout the observation period. Final weight records showed normal gain in all animals.

NECROPSY FINDINGS: Gross necropsy revealed no visceral abnormalities.

POTENTIAL TARGET ORGANS: None identified

SEX-SPECIFIC DIFFERENCES: None obvious from the report.

Conclusion : The rat oral LD50 for Alfol 12 was >26.53 g/kg with no obvious target organ identified.

Reliability : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Source : Scientific Associates Inc. 1965d
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference
11.08.2005

Vaishnav, D.D., Boethling, R.S., and Babeu, L. 1987. Quantitative structure-biodegradability relationships for alcohols, ketones and alicyclic compounds. Chemosphere 16(4): 695-703.
(22)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)</u>

Type : LD50

Species	:	rat
Strain	:	Wistar
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: aqueous suspension
Value	:	> 5000 mg/kg bw
Method	:	other: OECD 401 (limit dose)
Year	:	1981
GLP	:	yes
Test substance	:	dodecanol (112-53-8)
Test substance	:	Tradename Lorol 12
Test condition	:	TEST ORGANISMS: Rat (Wistar) - Source: Winkelmann, Hanover Germany - Weight at study initiation: males mean weight 156 g, females 136 g - Group size: 5M+5F - Controls: no ADMINISTRATION: gavage animals fasted - Doses: 5 g/kg - Doses per time period: single - Volume administered or concentration: 20 ml/kg of a 25% aqueous suspension. - Post dose observation period: 14 days EXAMINATIONS: Clinical signs were observed at 1, 4 and 24 hours after dosing and then daily thoughout the obsrvation period. Body weights were recorded immediately prior to dosing and at 24 hours, 1 week and two weeks after dosing. All survivors were subject to gross necropsy.
Result	:	MORTALITY: There were no deaths during the course of the study. CLINICAL SIGNS: Slight sedation and piloerection in all test animals during the first 24 hours after dosing. The animals gained in bodyweight at all measurement points during the observation period. NECROPSY FINDINGS: Nothing remarkable. POTENTIAL TARGET ORGANS: None identified SEX-SPECIFIC DIFFERENCES: None.
Conclusion	:	The rat oral LD50 for Lorol 12 applied as an aqueous suspension was >5 g/kg. Signs of intoxication were confined to mild sedation and

piloerection on the day of dosing. There were no gross histopathological changes and no evidence of specific target organ toxicity.

Reliability : (2) valid with restrictions
Guideline study
Source : Henkel KGaA 1981b
Hayes Consultancy Service Bromley, Kent
Flag : Critical study for SIDS endpoint
Reference Laboratory of Pharmacology and Toxicology. 1997. Examination of 1-Dodecanol in an acute immobilization test in Daphnia magna. LPT Report No. 10762/97.
11.08.2005 (12)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type : LD50
Species : other: rat, rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 10000 mg/kg bw
Method :
Year :
GLP :
Test substance : dodecanol (112-53-8)

Remark : The results from two acute oral studies are reported in Clayton and Clayton. The acute oral LD50 in rats is reported to be greater than 10.6 g/kg and 12.8 g/kg, and greater than 29.9 g/kg for rabbits. The animals that survived either 12.8 or 29.9 g/kg technical lauryl alcohol demonstrated no significant gross or microscopic changes.

Reliability : (4) not assignable
Secondary literature reference
Reference Henkel KGaA. 1992. 1-Dodecanol:
11.08.2005 Algen-Zellvermehrungshemmtest. Biological Research and Product safety/Ecology: Unpublished results; Report No. RE 920200.
(7)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Type: LD50
Species: rat

Strain: other: COX-SD
Sex: male/female
No. of Animals: 10
Vehicle: other: 50% w/w suspension in 1% w/w gum tragacanth
Doses: 7.26, 12.62, 15.89 and 20 g/kg
Value: > 20000 mg/kg bw

Method: other: contract laboratory protocol
Year: 1977
GLP: no data
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: MORTALITY:
- Time of death: Observation days 5 (dose level 12.62 g/kg), 6 and 10 (dose level 20 g/kg).
- Number of deaths at each dose: 0/10, 1/10, 0/10, 2/10 all deaths were amongst females.

CLINICAL SIGNS: Animals at each dose displayed the following: hypoactivity, diarrhea, hypersalivation, diuresis, ocular porphyrin deposits, unthriftiness, thinness, and emaciation. Surviving animals returned to normal between 1 and 10 days following dosage. All survivors showed weight gains within expected limits by the end of the observation period.

NECROPSY FINDINGS: Two animals which succumbed had moderate to severe congestion of the kidneys, adrenals, liver, lungs, stomach and gastrointestinal tract, haemorrhages (1 rat), and erosion of the mucosa of the stomach. The remaining decedent was in an advanced state of autolysis and no conclusions could be drawn. Of the animals that were sacrificed, gross necropsy findings were unremarkable.

POTENTIAL TARGET ORGANS: Erosion of the gastric mucosa was noted in 2 decedents.

SEX-SPECIFIC DIFFERENCES: Females appear rather more susceptible, mortalities were confined to the females.

Source: Scientific Associates, Inc. 1977b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: rat (COX-SD)
- Source: not reported
- Weight at study initiation: 210-299g
- Group size: 5M+5F fasted

- Controls: no

ADMINISTRATION: Gavage
- Doses: 7.26, 12.62, 15.89 and 20 g/kg (based on range finder)
- Doses per time period: single
- Volume administered or concentration: 50% suspension highest practical dose 20 g/kg.
- Post dose observation period: 14 days

EXAMINATIONS: The animals were observed for clinical signs of toxicity and death several times on the day of dosing and daily thereafter. All decedents and survivors were necropsied. Survivors were weighed at the end of the observation period.

Test substance: Tradename Alfol 14

Conclusion: The rat oral LD50 for Alfol 14 is >20 g/kg. Animals at all dose levels showed signs of intoxication following dosing these persisting from 1 to 10 days. Erosion of the gastric mucosa was observed in two decedents but not in survivors.

Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions. Well documented and conducted study.

Flag: Critical study for SIDS endpoint

Reference: Scientific Associates, Inc. 1977b. Acute oral toxcity (LD50) in rats, acute dermal toxicity (LD50) in rabbits, dermal irritation test in rabbits, eye irritation test in rabbits, and inhalation toxicity test in rats. ALFOL 14 alcohol.

16-JUL-2005 (64)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)</u>

Type: LD50
Species: rat
Strain: other: Carworth-Wistar rat
Sex: male
No. of Animals: 5
Vehicle: other: undiluted
Doses: not reported
Value: = 32500 ml/kg bw

Method: other: Smyth et al, 1962
Year: 1969
GLP: no
Test substance: other TS: Tetradecanol (mixed isomers)

Result: The rat oral LD50 for the mixed isomers of tetradecanol was 32.5 ml/kg (confidence limits 29.1 - 36.5). The density is not given in the publication but assuming a density of the order of 0.83 (from physical data included in this Iuclid) this gives an LD50 of 26.98 g/kg.

This value is also reported by Opdyke, 1975.

Source: Smyth et al. 1969

Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rat (Carworth-Wistar)
- Age: 5 weeks
- Group size: 5/group non-fasted
- Controls: no

ADMINISTRATION:
- Doses: not reported
- Doses per time period: single
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Mortality only. LD50 calculated using the methods of Weil (1952) and Thompson (1947).

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment. Study considered valid although result reporting is limited.

Flag: Critical study for SIDS endpoint

Reference: Opdyke, D.L.J. 1975 Fragrance raw material monographs - Alcohol C14 Myristic. 13 (Suppl.) 699-700.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

Smyth, H.F., Carpenter, C.P., Weil, C.S., Pozzani, U.C., Striegel, J.A., and Nycum, J.S. 1969. Range-finding toxicity data: List VII. Am. Ind. Hyg. Assoc. J. 30(5): 470-476.

16-OCT-2004 (53) (54) (68)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)</u>

Remark: Summary data reported in secondary references. Rat oral LD50 >5g/kg. Unpublished data Levenstein, 1972. No other details

provided. This appears to be the same reference reported in
Iuclid 2000 as Henkel unpublished report archive TBD 790109
(no. 232)
Source: Hayes Consultancy Service Bromley, Kent
Test substance: > 95% 1-Tetradecanol (112-72-1)
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau Tetradecanol Cas# 112-72-1.

Opdyke, D.L.J. 1975 Fragrance raw material monographs - Alcohol C14 Myristic. 13(Suppl.) 699-700

RTECS, 2004.
16-OCT-2004 (44) (53) (57)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Remark: Summary report, the LD50 in Holzman rats was reported as >8.0 g/kg. No further details available.
Source: Hayes Consultancy Service Bromley, Kent
Test substance: > 95% 1-Tetradecanol (112-72-1)
Reliability: (4) not assignable
Secondary reference.
Cosmetic Ingredient Review 1988 Final report on the safety assessment of cetearyl alcohol, cetyl alcohol, isostearyl alcohol, myristyl alcohol and behenyl alcohol. J. Am. Coll. Tox. 7(3): 359-413.
15-OCT-2004 (12)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: LD50
Species: rat
Strain: other: Sprague-Dawley CD
Sex: male/female
No. of Animals: 10
Vehicle: other: arachis oil
Doses: 2000 mg/kg
Value: > 2000 mg/kg bw

Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1996
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)
Result: MORTALITY: There were no deaths.

CLINICAL SIGNS: No clinical signs of systemic toxicity. All animals showed the expected body weight gain over the observation period.

NECROPSY FINDINGS: Unremarkable

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.

Source: Hempstock 1996a
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rat (Sprague-Dawley)
- Source: Charles River, Margate, Kent, UK
- Age: 5-8 weeks
- Weight at study initiation: males 135-145g, females 127 -137g
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION: Gavage
- Doses: Single dose level of 2000 mg/kg based on a range finding test.
- Doses per time period: single dose
- Volume administered or concentration: 10 ml/kg at a concentration of 200 mg/ml in arachis oil.
- Post dose observation period: 14 days

EXAMINATIONS: The rats were observed for clinical signs of toxicity and mortality 30 minutes, 1, 2 and 4 hours after dosing and thereafter daily throughout the observation period. Body weights were recorded prior to dosing on day 0 and then at 7 and 14 days. All animals were subject to gross pathological examination at the end of the observation period.

Test substance: Tradename Kalcol 6098

Conclusion: The rat oral LD50 for Kalcol 6098 is >2000 mg/kg. At this dose level there were no signs of toxicity.

Reliability: (1) valid without restriction
Guideline study.

Flag: Critical study for SIDS endpoint

Reference: Hempstock, C. 1996a. Kalcohl 6098: Acute oral toxicity (limit test) in the rat. SPL Project Number 140/495.

17-OCT-2004 (38)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Type: LD50

Species: rat
Strain: Wistar
Sex: male/female
No. of Animals: 10
Vehicle: other: olive oil
Doses: 5000 g/kg
Value: > 5000 mg/kg bw

Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1981
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: MORTALITY: All animals survived the observation period.

CLINICAL SIGNS: Slight sedation and piloerection were observed during the first 24 hours after dosing in all rats. The average body weight of the groups of male and female rats increased over the observation period.

NECROPSY FINDINGS: Unremarkable.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.
Source: Henkel KGaA 1981c
Hayes Consultancy Service Bromley, Kent
Test condition: TEST ORGANISMS: rat (Wistar)
- Source: Winkelmann, Hanover, Germany
- Weight at study initiation: average body weight males 174g, females 144g.
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION: gavage
- Doses: 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: 10 ml/kg as a 50% suspension in olive oil.
- Post dose observation period: 14 days.

EXAMINATIONS: Mortality and clinical signs were recorded. Body weights were taken before dosing and at 24 hours, 1 and 2 weeks after dosing. All rats were subject to gross necropsy at the end of the observation period.
Test substance: Tradename Lorol 16/Lanette 16

Conclusion: The rat oral LD50 for Lorol (Lanette) 16 is >5000 mg/kg. Clinical signs were confined to slight sedation and piloerection in the first 24 hours after dosing. Also reported in Iuclid 2000.
Reliability: (1) valid without restriction
Guideline study.
Flag: Critical study for SIDS endpoint
Reference: Henkel KGaA. 1981c. Hexadecanol: Evaluation of acute oral toxicity. Unpublished data, Report No. R 9500188 (944) and summary report 1999.

Iuclid 2000 European Commission - European Chemicals Bureau
Hexadecan-1-ol Cas# 36653-82-4.
17-OCT-2004 (39) (50)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: LD50
Species: rat
Strain: other: Holzman albino
Sex: male/female
No. of Animals: 5
Vehicle: other: 20% w/v suspension in corn oil
Doses: 2.00, 3.99 and 7.96 g/kg
Value: > 7960 mg/kg bw

Method: other: Standard contract laboratory procedure.
Year: 1965
GLP: no
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: MORTALITY: There were no mortalities at any dosage level tested.

CLINICAL SIGNS: Diarrhoea was observed at all dose concentrations during the first 24 hours after dosing. All animals appeared normal within 48-hours post-dosage. Weight gain was within the normal limits.

NECROPSY FINDINGS: Gross necropsy revealed no remarkable signs.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None.
Source: Scientific Associates, Inc. 1965e

Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rat (Holzman)
- Source: No reported
- Weight at study initiation: 204-254 g
- Group size: 5M+5F fasted
- Controls: No

ADMINISTRATION: gavage
- Doses: 2.00, 3.99 and 7.96 g/kg
- Doses per time period: single
- Volume administered or concentration: 20% suspension in cornoil
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs and mortality were recorded several times during the day of dosing and daily thereafter. All animals were necropsied and terminal body weights of survivors were recorded.

Test substance: Tradename Alfol 16
Tradename Alfol 16

Conclusion: The rat oral LD50 for Alfol 16 was >7.96 g/kg. The only clinical sign was diarrhoea at all dose levels in the first 24 hours after dosing. Gross necropsy revealed no remarkable changes. This study is reported in Iuclid 2000 erroneously giving the LD50 value as 7500 mg/kg.

Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Hexadecan-1-ol Cas# 36653-82-4

Scientific Associates, Inc. 1965e. Acute oral toxicity (LD50) study in rats. ALFOL 16.
17-OCT-2004 (50) (76)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Remark: Summary report. Mouse oral LD50 3200 mg/kg, no further details available. Also reported in Iuclid 2000.

Test substance: 1-hexadecanol (36653-82-4)

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Hexadecan-1-ol Cas# 36653-82-4.

Opdyke, D.L.J. 1978 Fragrance raw materials monographs Fd. Cos. Tox. 16: 683-686.

18-OCT-2004 (50) (66)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Remark: Summary report of unpublished data provided by Fassett, originally reported in Patty's 2nd edition, 1963. Rat oral LD50 6.4-12.8 g/kg, mouse oral LD50 3.2-6.4 g/kg. No further details available.
Test substance: Cetyl alcohol, described in Patty, 1963 as a synthetic liquid C16 alcohol that may have contained impurities.
Reliability: (4) not assignable
Secondary reference.
Reference: Opdyke, D.L.J. 1978 Fragrance raw materials monographs Fd. Cos. Tox. 16: 683-686.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

Patty, F.A (ed) 1963 Industrial Hygiene and Toxicology 2nd revised edition Vol. 11 Toxicology Chapter 34 Alcohols (J.F. Treon) Interscience publishers.
06-AUG-2005 (66) (67) (68)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Type	:	LD50
Species	:	rat
Strain	:	Wistar
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: 50% suspension in DMSO
Value	:	> 5000 mg/kg bw
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	1981
GLP	:	yes
Test substance	:	octadecanol (112-92-5)
Test substance	:	Tradename Lorol/Lanette 18
Test condition	:	TEST ORGANISMS: rat (Wistar) - Source: Winkelmann, Hanover, Germany - Weight at study initiation: average body weight males 177g, females 141g. - Group size: 5M+5F fasted - Controls: no

ADMINISTRATION: gavage
- Doses: 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: 10 ml/kg as a 50% suspension in DMSO.
- Post dose observation period: 14 days.

EXAMINATIONS: Mortality and clinical signs were recorded. Body weights were taken before dosing and at 24 hours, 1 and 2 weeks after dosing. All rats were subject to gross necropsy at the end of the observation period.

Result : MORTALITY: All animals survived the observation period.

CLINICAL SIGNS: Directly after application the animals showed moderate piloerection and slight sedation. These effects vanished completely within 24 hours. Group body weights increased over the observation period.

NECROPSY FINDINGS: Round deposits of test substance remained in the stomach. There were no other gross pathological observations.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None.

Conclusion : The rat oral LD50 for Lorol (Lanette) 18 was >5000 mg/kg. Signs of intoxication were confined to transient mild sedation and moderate piloerection.

Reliability : (1) valid without restriction
Guideline study

Source : Henkel KGaA 1981g
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Henkel KGaA. 1981g. Octadecanol: Evaluation of acute oral toxicity. Unpublished data, Report No. R 9500191 and summary dated 1999.

11.08.2005 (12)

<u>1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)</u>

Type : LD50
Species : rat
Strain : other: Holzman
Sex : male/female
Number of animals : 5

Vehicle : other: 20% w/v corn oil suspension
Value : > 7960 mg/kg bw
Method : other: contract laboratory protocol.
Year : 1965
GLP : no
Test substance : octadecanol (112-92-5)

Test substance : Tradename Alfol 12

Test condition : TEST ORGANISMS: Rat (Holtzman)
- Weight at study initiation: 205-254 g
- Group size: 5M+5F no indication as to whether the animals were fasted.
- Controls: No

ADMINISTRATION: GAvage
- Doses: 2.0 and 7.96 g/kg
- Doses per time period: single
- Volume administered or concentration: 20% suspension in corn oil.
- Post dose observation period: 14 days

EXAMINATIONS: Mortality and clinical signs frequently on day of dosing, thereafter daily. Bodyweights were recorded at study initiation and at the end of the observation period. Gross necrospy was carried out on all animals at the end of the observation period.

Result : MORTALITY: There were no mortalities at any dose level.

CLINICAL SIGNS: No signs of toxicity or pharmacological effects were observed at the low test level. Diarrhoea was observed in most animals at the higher dose level at 24 hours. All animals appeared normal within 48 hours. All animals gained weight within the normal limits.

NECROPSY FINDINGS: Gross necropsy of the animals sacrificed at termination did not reveal any remarkable findings.

POTENTIAL TARGET ORGANS: None identified.
SEX-SPECIFIC DIFFERENCES: None reported.

Conclusion : The rat oral LD50 of Alfol 18 is >7960 mg/kg. Other than diarrhoea at the top dose level there were no clinical or gross pathological signs toxicity.

Reliability : (2) valid with restrictions
Study well documented, meets generally accepted scientific

principles, acceptable for assessment.

Source : Scientific Associates, Inc. 1965f
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Scientific Associates, Inc. 1965f. Acute oral toxicity (LD50) study in rats. Alfol 18.

11.08.2005 (21)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Type : LD50
Species : rat
Strain : other: Sprague-Dawley CD
Sex : male/female
Number of animals : 10
Vehicle : other: arachis oil
Value : > 2000 mg/kg bw
Method : OECD Guide-line 401 "Acute Oral Toxicity"
Year : 1996
GLP : yes
Test substance : octadecanol (112-92-5)

Test substance : Tradename Kalcol 8098

Test condition : TEST ORGANISMS: Rat (Sprague-Dawley)
- Source: Charles River, Margate, Kent, UK
- Age: 5-8 weeks
- Weight at study initiation: males 135-145g, females 127 -137g
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION: Gavage
- Doses: Single dose level of 2000 mg/kg based on a range finding test.
- Doses per time period: single dose
- Volume administered or concentration: 200 ml/kg at a concentration of 10mg/ml in arachis oil. Preparation of the solution was aided by warming in a water bath.
- Post dose observation period: 14 days

EXAMINATIONS: The rats were observed for clinical signs of toxicity and mortality at 30 minutes, 1, 2 and 4 hours after dosing and thereafter daily throughout the observation period. Body weights were recorded prior to dosing on day 0 and then at 7 and 14 days. All animals were subject to both pathological examination at the end of the observation period.

Result : MORTALITY: There were no deaths.

CLINICAL SIGNS: No clinical signs of systemic toxicity. All animals showed the expected body weight gain over the observation period.

NECROPSY FINDINGS: Unremarkable

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.

Conclusion : The rat oral LD50 fro Kalcol 8098 is >2000 mg/kg. There were no signs of toxicity.

Reliability : (1) valid without restriction
Guideline study

Source : Hempstock 1996b
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Hempstock, C. 1996b. Kalcohl 8098: Acute oral toxicity (limit test) in the rat. SPL Project Number 140/501.

11.08.2005 (10)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Type: LD50
Species: rat
Strain: Sprague-Dawley
Sex: male/female
No. of Animals: 20
Vehicle: other: 0.8% hydroxypropyl-methylcellulose gel
Doses: 8250 and 10000 mg/kg
Value: > 10000 mg/kg bw

Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1987
GLP: yes
Test substance: >= 90% 1-eicosanol (629-96-9)
Result: MORTALITY: All animals survived the 14 day observation period.

CLINICAL SIGNS: No clinical signs of toxicity. There was no adverse effect on food intake or bodyweight gain.

NECROPSY FINDINGS: Unremarkable.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None

Source: Laboratory of Pharmacology and Toxicology 1987a
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rat (Sprague-Dawley)
- Source: Lippische Versuchtierzucht, Hagemann GmbH, Extertal, Germany
- Age: 42-50 days
- Weight at study initiation: 156-168 g
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION: Gavage
- Doses: 8250 and 10,000 mg/kg
- Doses per time period: single
- Volume administered or concentration: prepared using 0.8% hydroxypropyl-methylcellulose gel, dose concentration/volume not reported.
- Post dose observation period: 14 days

EXAMINATIONS: Mortality, food and water consumption and weight gain were monitored during the observation period. All animals were subject to gross pathological examination.

Test substance: Tradename Nacol 20

Conclusion: The rat oral LD50 for Nacol 20 is >10g/kg. At this dose level there was no evidence of toxicity in any of the parameters monitored. Reported in Iuclid 2000.

Reliability: (1) valid without restriction
Guideline study.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau
Icosan-1-ol Cas# 629-96-9.

Laboratory of Pharmacology and Toxicology. 1987a. Acute oral toxicity of Nacol 20 in Sprague-Dawley rats.

05-AUG-2005 (10) (12)

<u>1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)</u>

Type: LD50
Species: rat
Strain: no data
Sex: male
No. of Animals: 5

Vehicle: no data
Doses: no data
Value: > 64 ml/kg bw

Method: other: Smyth et al, 1962
Year: 1969
GLP: no data
Test substance: other TS: icosanol mixed isomers

Result: The rat oral LD50 for the mixed isomers of icosanol is > 64 ml/kg (>53760 mg/kg using the density of 0.84 g/cm3 reported in chapter 2.3).
Source: Smyth, 1969
Test condition: TEST ORGANISMS: Rat (Carworth-Wistar)
- Age: 5 weeks
- Group size: 5/group non-fasted
- Controls: no

ADMINISTRATION:
- Doses: not reported
- Doses per time period: single
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Mortality only. LD50 calculated using the methods of Weil (1952) and Thompson (1947).
Reliability: (2) valid with restrictions
Meets generally accepted scientific principles, acceptable for assessment. Study considered valid although result reporting is limited. Rats were non-fasted. This study is also reported in Patty 2001.
Reference: Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

Smyth, H.F., Carpenter, C.P., Weil, C.S., Pozzani, U.C., Striegel, J.A., and Nycum, J.S. 1969. Range-finding toxicity data: List VII. Am. Ind. Hyg. Assoc. J. 30(5): 470-476.
11-MAY-2006 (17) (19)

<u>1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)</u>

Type: LD50
Species: rat
Strain: Sprague-Dawley
Sex: male/female

No. of Animals: 6
Vehicle: other: suspension in arachis oil
Doses: 2000 mg/kg
Value: > 2000 mg/kg bw

Method: OECD Guide-line 423
Year: 1997
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)

Result: MORTALITY: There were no deaths.

CLINICAL SIGNS: No clinical signs of systemic toxicity. All animals showed the expected body weight gain over the observation period except for one female which showed a weight loss during the second observation week. This was considered unlikely to be a toxicological effect.

NECROPSY FINDINGS: Unremarkable

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None considered of significance.
Source: Hempstock, 1997c
Hayes Consultancy Service Bromley, Kent
Test condition: TEST ORGANISMS: Rat (Sprague-Dawley-CD)
- Source: Charles River, Margate, Kent, UK
- Age: 8-12 weeks
- Weight at study initiation: males 217-246g, females 206-223g
- Group size: 3M initially followed when it appeared the males would survive by 3F, fasted
- Controls: no

ADMINISTRATION: Gavage
- Doses: Single dose level of 2000 mg/kg
- Doses per time period: single dose
- Volume administered or concentration: 10 ml/kg at a concentration of 200 mg/ml in arachis oil.
- Post dose observation period: 14 days

EXAMINATIONS: The rats were observed for clinical signs of toxicity and mortality 30 minutes, 1, 2 and 4 hours after dosing and thereafter daily throughout the observation period. Body weights were recorded prior to dosing on day 0 and then at 7 and 14 days. All animals were subject to gross pathological examination at the end of the observation period.
Test substance: Tradename Kalcol 220-80
Conclusion: The rat oral LD50 for Kalcol 220-80 is >2000 mgkg. There were

no signs of intoxication and no remarkable findings on gross necropsy.

Reliability: (1) valid without restriction
Guideline study.

Flag: Critical study for SIDS endpoint

Reference: Hempstock, C. 1997c. Kalcol 220-80: Acute oral toxicity study in the rat - acute toxic class method. SPL Project Number: 140/270.

06-AUG-2005 (12)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Type: LD50
Species: rat
Strain: Sprague-Dawley
Sex: male/female
No. of Animals: 10
Vehicle: other: 0.8% hydroxypropyl-methylcellulose gel
Doses: 8250 and 10000 mg/kg
Value: > 10000 mg/kg bw

Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1987
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)

Result: MORTALITY: All animals survived the 14 day observation period.

CLINICAL SIGNS: No clinical signs of toxicity. There was no adverse effect on food intake or bodyweight gain.

NECROPSY FINDINGS: Unremarkable.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None

Source: Laboratory of Pharmacology and Toxicology 1987b
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rat (Sprague-Dawley)
- Source: Lippische Versuchtierzucht, Hagemann GmbH, Extertal, Germany
- Age: 42-50 days
- Weight at study initiation: 157-167 g
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION: Gavage
- Doses: 8250 and 10,000 mg/kg
- Doses per time period: single

- Volume administered or concentration: prepared using 0.8% hydroxypropyl-methylcellulose gel, dose concentration/volume not reported.
- Post dose observation period: 14 days

EXAMINATIONS: Mortality, food and water consumption and weight gain were monitored during the observation period. All animals were subject to gross pathological examination.

Test substance: Tradename Nacol 22RD

Conclusion: The rat oral LD50 for Nacol 22 RD is >10g/kg. At this dose level there was no evidence of toxicity in any of the parameters monitored. This value is also reported in Iuclid 2000.

Reliability: (1) valid without restriction
Guideline study.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Docosan-1-ol Cas# 661-19-8.

Laboratory of Pharmacology and Toxicology. 1987b. Acute toxicity-oral-of NACOL 22 RD in Sprague-Dawley rats.

06-AUG-2005 (17) (19)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Type: LD50
Species: mouse
Strain: other: CF1
Sex: no data
No. of Animals: 10
Vehicle: other: olive oil
Doses: 1000 mg/kg
Value: > 1000 mg/kg bw

Method: other
Year: 1977
GLP: no data
Test substance: >95% 1-docosanol (661-19-8)

Remark: Summary report of an unpublished study from Henkel, 1977. A group of 10 mice (average wt. 25g) received a single dose of 1000 mg/kg in olive oil (heated) by stomach tube. None of the test animals died during the 8 day observation period. No further details available.

Reliability: (4) not assignable
Secondary reference.

Reference: Cosmetic Ingredient Review (CIR) 1988 Final report on the

safety assessment of cetearyl alcohol, cetyl alcohol, isostearyl alcohol, myristyl alcohol and behenyl alcohol. J. Am. Coll. Tox. 7(3):359-413.

06-AUG-2005 (9)

1-Tetracosanol, 1-Hexacosanol, 1-Octacosanol, and 1-Triacontanol for their respective Aluminum Salts

Type	:	LD50
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	80
Vehicle	:	other: gum arabic - water suspension
Value	:	> 5000 mg/kg bw
Method	:	other
Year	:	1995
GLP	:	no data
Test substance	:	C24-C30 alcohols
Test condition	:	TEST ORGANISMS: Rat, Sprague-Dawley - Source: National Centre for the Production of Laboratory Animals, Cuba - Age: Not reported - Weight at study initiation: 150 - 200g - Group size: 8 males + 8 females per group - Controls: Yes, vehicle only ADMINISTRATION: Oral - Doses: 0, 500, 1500, 2500 and 5000 mg/kg - Doses per time period: single - Volume administered or concentration: Animals received similar volumes of the vehicle. - Vehicle: 10 mg/ml gum arabic in water. - Post dose observation period: 14 days EXAMINATIONS: Observations of clinical signs were made hourly in the first 4 hours after dosing, 4 hourly thereafter to 24 hours and then daily. Bodyweights were recorded at the start and finish of the experiment. At the end of the observation period, blood samples were taken for haematological and biochemical analyses of haemoglobin, haematocrit, GOT amd GPT, alkaline phosphatase, creatinine and glucose. All animals were subject to gross histopathological examination and organ weights (liver, kidneys, heart, spleen, lungs and thymus) were recorded. Histopathological examination was carried out on all top dose and control rats.

STATISTICAL ANALYSIS: Biochemical and haematological parameters and organ weights were analysed using variance analysis (ANOVA) and carried out independently for each sex. Analysis of mortality and frequency of histopathological signs were conducting using the Fischer Exact Proportions TEst.

Result : MORTALITY:
- Time of death: All rats survived the 14 day observation period. LD50 >5000 mg/kg

CLINICAL SIGNS: There were no signs of toxicity. Increase in bodyweight was similar between treated and control groups and there were no statistical differences.

HAEMATOGLOGY AND BIOCHEMISTRY: No statistically significant changes attributable to treatment.

NECROPSY FINDINGS: No remarkable changes in gross or microscopic pathology. No significant changes in the weight of the major organs weighed.

POTENTIAL TARGET ORGANS: None identified

SEX-SPECIFIC DIFFERENCES: None identified

Conclusion : The rat oral LD50 for sample D-002 is >5000 mg/kg. There were no mortalities or other adverse effects on any of the parameters monitored.

Reliability : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment. Although not reported as being carried out to any specific regulatory guideline the conduct of the study appeared to similar to that required for a guideline study and the publication provided a good level of detail.

Flag : Critical study for SIDS endpoint

Reference Rodeiro, I. et al 1995 Toxicologia aguda oral del D-002 en ratas Sprague Dawley. Revista CENIC Ciencias Biologicas 26 (1-3): 34-36 (translation available).

10.08.2005 (5)

<u>1-Tetracosanol, 1-Hexacosanol, 1-Octacosanol, and 1-Triacontanol for their respective Aluminum Salts</u>

Method	:	
Year	:	
GLP	:	
Test substance	:	C24-C30 alcohols
Remark	:	Unpublished data provided by Rodeiro, 1996 giving LD50 values in mice, rabbits and dogs. All three species showed no measurable toxicity at dose levels of up to 5000 mg/kg.
Reliability	:	(4) not assignable Citation of unpublished results, no further details available.
Reference		Rodriguez, MD, R Gamez, M Sanchez and H Garcia. 1998. Developmental Toxicity of D-002 (a Mixture of Aliphatic Primary Alcohols) in Rats and Rabbits. Journal of Applied Toxicology, 18, 313-316.
11.04.2005		(8)

5.1.2 Acute Inhalation Toxicity

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LC50
Value	> 60000 ppm
Species	Mouse
Strain	CD-1
Sex	male/female
Number of animals	6
Vehicle	
Doses	40,000, 50,000 and 60,000 ppm
Exposure time	60 minute(s)
Method	other
Year	1985
GLP	no data
Test substance	other TS: 95% USP ethanol (64-17-5)
Remark	The sexes of the animals were not specified and the numbers given are estimates as 12 animals per exposure concentration were used. Time of death: Not applicable. no deaths. Description, severity, time of onset and duration of clinical signs at each dose level: Slight to moderate ataxia occurred and recovery time was more than 4 hours at all exposure levels. Necropsy findings: Not applicable Potential target organs: Not applicable.

Result	Sex comparison: Not applicable No LC50 was determined as no deaths occurred at any of the exposure concentrations. Slight to moderate ataxia was observed and recovery from this exceeded 4 hours at all exposure levels. Necropsy and target organ study not applicable.
Test condition	Age of animals: Not stated but weighed 25~30 g. Animals were caged with wood~chip bedding in a room at a temperature of 22-24 deg. C and 121 hr Iight/12 hr dark cycle. Doses: 40,000, 50,000 and 60,000 ppm for different exposure duration. Doses per time period: One exposure pereiod per exposure level. Volume administered or concentration: Not applicable. Post dose observation period: 72 days. Exposure duration: 60, 30 and 10 minutes.
Reliability	(2) valid with restrictions The study is reasonably well reported but there are the following deviations from an ideal protocol. Exposure period only 60 minutes. Species mouse rather than preferred rat. Observations reported for only 3 days rather than 14. Volume of chamber 29 litres (above 20 litres) No detailed observations of effects. No pathology No detailed reporting of findings down to individual animal.
Flag	Critical study for SIDS endpoint
Reference	Moser, V. and Balster (1985). Acute motor and lethal effects of inhaled toluene, 1,1,1-trichloroethane, halothane and ethanol in mice: effects of exposure duration. Toxicol. Appl. Pharmacol. 77: 285-291.
12.11.2004	(169)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	LCLo
Value	> 29.43 mg/l
Species	Rat
Strain	Other
Sex	no data
Number of animals	12
Vehicle	
Doses	saturated air
Exposure time	7 hour(s)
Method	other

Year	1981
GLP	no
Test substance	ethanol (64-17-5)
Remark	12 rats were exposed to a saturated vapour concentration of the test substance at a temperature of 20 degrees C. There were no deaths. The mean atmospheric concentration of test substance was 29.43mg/l. BASF Test
Reliability	4) not assignable
Reference	BASF AG Toxicology Department unpublished research. (80/30) 23-12-1981.
12.11.2004	(170)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Other
Value	
Species	Mouse
Method	other
Year	1982
GLP	no data
Test substance	ethanol (64-17-5)
Remark	13,300 ppm for 1.33 hours caused ataxia. 23,940 ppm for 1.25 hours caused narcosis. 29,300 ppm for 7 hours caused narcosis and deaths. 31,900 ppm for 0.33 hours caused ataxia.
Reliability	(4) not assignable
Reference	Lehmann, K.B. & Flury, F. (1938) Toxicol. Hyg. Tech. Losung. Springer. Berlin. cited in Patty (1982) loc. cit.
18.11.2004	(171)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Other
Value	
Species	Rat
Exposure time	7 hour(s)
Method	other
Year	1982
GLP	No
Test substance	ethanol (64-17-5)
Remark	12 rats were exposed to a saturated atmosphere of the test

	substance at 20 degrees C for seven hours. No deaths resulted. 50% ethanol in water BASF test.
Reliability	(4) not assignable
Reference	BASF AG Toxicology Department unpublished research (80/95) 19-01-1982.
12.11.2004	(172)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LC50
Value	= 5.9 mg/l
Species	Rat
Strain	
Sex	6 hour(s)
Method	other
Year	1980
GLP	No
Test substance	ethanol (64-17-5)
Remark	BASF test
Reliability	(4) not assignable
Reference	BASF AG Toxicology Department unpublished research. (80/30) 14-10-1980.
12.11.2004	(173)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LC50
Value	= 124.7 mg/l
Species	Rat
Exposure time	4 hour(s)
Method	other
Year	1980
GLP	No
Test substance	ethanol (64-17-5)
Remark	BASF test
Reliability	(4) not assignable
Reference	BASF AG Toxicology Department unpublished research. (80/30) 13-11-1980.
12.11.2004	(174)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LCO
Value	16000 ppm

Species	Rat
Exposure time	8 hour(s)
Method	other
Year	no data
GLP	ethanol (64-17-5)
Test substance	
Remark	Patty's Toxicology of Indiustrial Chemicals
Reliability	(4) not assignable
Reference	Unpublished data from the Carnagie-Mellon Institute of Research cited in Patty (1982) loc. cit.
29.09.2003	(175)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Other
Value	
Species	Rat
Exposure time	8 hour(s)
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	No details of method. Some deaths occurred at 16000 ppm and at 32000 ppm.
Reliability	(4) not assignable .
Reference	Smyth. H.F. Jr. (1956) Am. Ind. Hyg. Assoc. Q. 17. 129. cited in Patty (1982) loc. cit.
12.11.2004	(176)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Other
Value	
Species	Rat
Method	other
Year	1918
GLP	No
Test substance	ethanol (64-17-5)
Remark	Duration of exposure varied from 0.5 to 21.75 hours. No effects at 3260 ppm for 6 hours but drowsiness by 8 hours. Incoordination at 5660 ppm for 1.75 hours and light narcosis at 6400 ppm for 12 hours. At 12,400 to 12,700 ppm there was deep narcosis by 8.5 hours and deaths by 21.75 hours. Deep narcosis and death occurred at 44,000 ppm by 6.5 hours.

Reliability	(4) not assignable
Reference	Loewy, A. & von der Heide, R. (1918) Ueber die Aufnahme des Aethylalkohols durch die Atmung. Biochem. Z. 86, 125 - 175.
12.11.2004	(177)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Other
Value	
Species	guinea pig
Method	other
Year	
GLP	No
Test substance	ethanol (64-17-5)
Remark	Duration of exposure varied from 3.75 to 24 hours. No overt effects at 6400 ppm for 8 hours or 9080 ppm for 5.25 hours. Light narcosis and incoordination at 12,850 to 13,300 ppm for 8.75 to 24 hours. No effects at 19,260 ppm for 3.75 hours, but 20,000 ppm for 6.5 hours caused incoordination, and 21,900 ppm for 9.8 hours caused deep narcosis and death.
Reliability	(4) not assignable
Reference	Loewy, A. & von der Heide, R. (1918) Ueber die Aufnahme des Aethylalkohols durch die Atmung. Biochem. Z. 86, 125 - 175.
12.11.2004	(177)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LC50
Value	= 39 mg/l
Species	Mouse
Exposure time	4 hour(s)
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Reliability	(4) not assignable
Reference	Anon. (1982) Gig. Truda prof. Zabol. 26, 53. cited in RTECS (1992) loc. cit.
12.11.2004	(178)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Other

Value	
Species	guinea pig
Strain	Hartley
Sex	Male
Number of animals	
Vehicle	other: 0.9% saline
Doses	concentration 31, 62,5, 125, 250mM
Exposure time	
Method	other
Year	1994
GLP	no data
Test substance	ethanol (64-17-5)
Method	Animals with tracheas cannulated with polyethylene tubes, artificially ventilated (tidal voI10ml/kg). Changes to resistance to inflation measured by pressure required to overinflate by 2x tidal volume for 2 breaths. Animals subjected to 15mins saline aerosol, followed by 15second bursts of ethanol containing aerosol, with a 5 minute gap before next burst of ethanol aerosol, with increasing concentrations used. 46.4% of aerosol measured as deposited in lungs by radiolabel technique.
Remark	Study designed to assess if ethanol in aerosol form causes bronchoconstriction. Ethanol did not cause bronchorestriction.
Reliability	(4) not assignable
Reference	Myou S, Fujimura M, Bando T, Saito M, Matsuda T (1994) Aerosolized acetaldehyde, but not ethanol, induces histamine mediated brochoconstriction in guinea pigs. Clin Exp Allergy, 24, 140-3.
18.11.2004	(179)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	other: volunteer study
Value	
Species	Human
Strain	
Sex	male/female
Number of animals	6
Vehicle	other: saline
Doses	0, 25% in aerosol form
Exposure time	30 minute(s)
Test substance:	ethanol (64-17-5)
Method	Volunteers: Healthy; 2 atopic, 5 non-atopic; 4 women, 2 men;

	5 nonsmokers, 1 regular smoker; age 2845yrs. Inhalation via the mouth of an aerosol, particle size 0.5-4.0um. 5 day interval between exposures. Lung function assessed by recording partial and maximum expiratory flow volume at time zero and repeatedly during the 4 hrs after exposure (1 sec forced expiratory volume and flow rate at 40% of the forced vital capacity.) Mean of three repeats used. Statistical analysis: student's t test. Ethanol concentrations were measured using Draeger tubes in inhaled (measured in breathing tube) and expired air (5 & 30 mins after exposure.)
Remark	Subjects reported coughing at start of exposure and 3 reported chest tightness at end. None reported signs of intoxication normally associated with ethanol ingestion. No symptoms were experienced with the saline control. Ethanol decreased the maximum expiratory flow rates for the whole of the 4 hour period after exposure (8-37% statistically significant reduction for the first 90 minutes after exposure.) There was no significant effect on the one second forced expiratory volume. The ethanol concentration in inspired air was 0.18-0.2% (1800-2000ppm) and in exhaled air for 30 minutes post exposure 0.06-0.1 % (600-1000ppm)
Reliability	(4) not assignable
Reference	Zuskin E, Bouhuys A, Sarie M (1981) Lung function changes by ethanol inhalation, Clin. Allergy, 11, 243-8.
18.11.2004	(180)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Other
Value	
Species	Mouse
Strain	C57BL
Sex	Female
Number of animals	
Vehicle	
Doses	single group exposed to 25-38 mg/l
Exposure time	24 hour(s)
Method	other
Year	1986
GLP	no data
Test substance	ethanol (64-17-5)
Method	Animals 12-24 weeks old. Caged mice placed in perspex inhalation chambers.

	Feed: CRM pellets (K&K Greefe), freely available during exposure. Aged matched control mice used Blood obtained in heparinised syringes (cardiac puncture) then mixed with EDTA. Hb, RBC and WBC determined by Coulter counter. PVC measured using microhaematocrit tubes. Platelet count determined (after 100x dilution in formal citrate) using a Neubauer counting chamber. Reticulocytes counted on unfixed smears of supervitally - stained blood. Blood films stained by the May-Grunwald-Giemsa method and differential leucocyte counts performed on 500 consecutive nucleated cells. Femoral marrow expekked into heparinised Hank's solution, dispersed into a single cell suspension and used for determination of marrow cellularity or deoxyuridine suppression values. Quantification of granulocyte-macrophage progenitor cells: Femoral marrow expelled into MEM alpha medium. Samples dispersed into single cell medium, washed twice, assays of CFU-GM performed on each marrow cell suspension in triplicate. Details of procedure given in reference.
Result	Many mice showed locomotor depression and ataxia. Blood ethanol levels were in the range 150-560mg/dl. Ethanol exposed mice developed leucopenia, neutropenia, lymphopenia, monocytopenia, thrombocytopenia but not anaemia or macrocytosis. There was no effect on deoxyuridine suppression values or number of granulocyte-macrophage progenitor cells. There was a slight reduction in the number of megakaryocytes.
Reliability	(4) not assignable
Reference	Malik F, Wickramasinghe (1986) Haematological abnormalities in mice continuously exposed to ethanol vapour. Br J. Exp. Path. 67, 831-8.
12.11.2004	(181)

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Test substance:	1-Butanol, Union Carbide sample procured 12/20/48 from Fellowship 155.
Method:	Method/guideline followed: Internal Union Carbide method for inhalation
Test type:	Acute inhalation.
GLP:	No

Year performed:	Not specified.
Species/strain:	Rat, albino Sherman
Sex: Female.	
Number of animals/ sex/dose:	6 females/dose x one dose (saturation - calculated saturated vapour concentration approximately 7200 ppm @ 20 degrees C).
Vehicle:	Air.
Route of admin.:	8 hour exposure to substantially saturated vapor produced by aeration of n-butanol at room temperature.
Results:	All animals survived and gained weight normally during the 14day observation period.
Comments:	At the end of the exposure, the only symptoms of distress were poor coordination or prostration.
Data quality:	Reliability: Key study. Klimisch quality 2.
Reference:	Union Carbide Corp. Bushy Run Research Center, Project Report No.14-73. Export, PA. 1951.

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Test substance:	1-Butanol, Union Carbide sample number A1939.
Method:	Method/guideline followed: Internal Union Carbide method for inhalation exposure.
Test type:	Acute inhalation.
GLP:	No
Year performed:	Not specified.
Species/strain:	Rat, albino Sherman
Sex:	
Number of animals/ sex/dose:	6 males/dose x one dose (8000 ppm).
Vehicle:	Air.
Route of admin.:	4 hour exposure to 8000 ppm n-butanol.
Results:	LC50 > 8000 ppm.
Comments:	All animals survived and gained weight normally during the 14 day observation period. At the end of the exposure, no. symptoms of distress were noted. The rats were normal.
Data quality:	Reliability: Key study. Klimisch quality 2.

Reference: Union Carbide Corp. Bushy Run Research Center, Project Report No.14-73. Export, PA. 1951.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species/strain: Mouse
Test method: Not Stated
GLP: No

Test results: 650 ppm, 7-hours, no evidence of toxicity 6600 ppm, 2-hours, signs of CNS depression.
Comments:
Reference: Patty, F.A. 1982. Industrial Hygiene and Toxicology, 3rd ed., New York, Chichester, Brisbane, Toronto, Singapore, Wiley-Interscience. IIC: 4571-4578. As cited in World Health Organization (WHO). 1987. Environmental Health Criteria 65:
Butanols Four Isomers: 1-Butanol 2-Butanol tert-Butanol Isobutanol. WHO.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species/strain: Male Wistar rats; mouse (strain not specified)
Test method: 4hr. Dynamic inhalation to n-butyl alcohol or 4hr. Dynamic inhalation to a 50Vol-% mixture of 1-butanol and m-xylene.
GLP: No

Test results: EC50 = 6530 ppm, rat ED50 3010 ppm, mouse

Comments: EC50 = The medial effective concentration which caused rotarod performance disturbances.
ED50 = The concentration which caused a 50% reduction in respiratory rate.
Reference: Korsak, Z, Swiercz, R. and Jedrychowski R. Effects of Acute Combined Exposure to n-ButylAlcohol and m-Xylene. Polish Jor. of Occup. Med. and Environmental Health. 6(1):35-41, 1993.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species/strain: Scs:CF-l male mice.
Test method: ASTM E981-84, 1984

GLP: No

Test results: RD50 = 233 ppm
RD50 = 11,696 ppm
Data Quality: Klimisch rating of 4 due to lack of original source documents
Reference: Registry of Toxic Effects of Chemical Substances. p. 1301 1985-86.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LC50
Species: rat
Strain: other: COX-SD
Sex: male/female
No. of Animals: 10
Vehicle: other: atmosphere generated as a mist
Doses: 21 mg/l
Exposure time: 1 hour(s)
Value: > 21 mg/l

Method: other: in house protocol
Year: 1977
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: MORTALITY: All animals survived the 14 day observation period.

CLINICAL SIGNS: During exposure all animals showed hypoactivity and/or ataxia, lethargy and prostration. However within 2 hours of removal from the exposure chamber the animals all appeared and continued to appear normal throughout the observation period. Final bodyweights showed a slight weight loss in one animal however the others all exhibited weight gains within expected limits.

NECROPSY FINDINGS: Gross necropsy revealed moderate pulmonary, adrenal and hepatic congestion in one animal only. The findings in the remaining 9 test animals were unremarkable.

POTENTIAL TARGET ORGANS: None identified.
Source: Scientific Associates, Inc. 1977c
Hayes Consultancy Service Bromley, Kent
Test substance: Tradename Alfol 6
Conclusion: The rat inhalational LC50 following a 1 hour exposure to a mist of Alfol 6 was >21 mg/l.
Test condition: TEST ORGANISMS: Rat (COX-SD)
- Source: not reported.
- Weight at study initiation: 245-356g
- Number of animals: 5m+5F/dose level

- Controls: none

ADMINISTRATION: inhalation, whole body exposure.
- Type of exposure: the atmosphere was generated as a mist, following exposure the animals were washed to remove any accumulated test material.
- Concentrations: 0.21 mg/l for 1 hour (not monitored)
- Particle size: Droplet size not reported
- Type or preparation of particles: The mist was generated using a nebuliser.
- Postexposure period: 14 days

EXAMINATIONS: The animals were observed frequently on the day of exposure and daily thereafter. Survivors were weighed and necropsied at the end of the exposure period.

Reliability: (2) valid with restrictions
Study well documented meeting generally accepted scientific principles, acceptable for assessment. Only one dose level, short exposure period, no indication of droplet size.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3

Scientific Associates, Inc. 1977c. Acute oral toxicity (LD50) in rats; Acute dermal toxicity (LD50) in rabbits, Dermal irritation test in rabbits; Eye irritation test in rabbits; Inhalation toxicity tests in rats: ALFOL 6. S.A. Number 233619.

12-SEP-2004 (29) (62)

<u>1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)</u>

Type: LC50
Species: rat
Strain: Sherman
Sex: male
Exposure time: 8 hour(s)

Method: other: screening
Year: 1951
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Result: The 8 hour LC50 of n-hexanol is greater than the substantially saturated vapour concentration. No rats died during this exposure.

Test condition: Groups of 6 rats were exposed to the substantially saturated vapours of n-hexanol generated by passing air through a disc bubbler at room temperature for up to 8 hours. There was no measurement of vapour concentration.
Reliability: (4) not assignable
Summary data on a number of substances, reporting limited. No measurement of vapour concentration.
Reference: Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

Smyth, H.F., Carpenter, C.P., and Weil, C.S. 1951. Range-finding toxicity data: List IV. A.M.A. Archives of Industrial Hygiene and Occupational Medicine 4:119-122.
12-SEP-2004 (48) (68)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LC50
Species: other: rat, mouse, guinea pig
Value: > 1060 ppm

Method: other: no data
Year: 1975
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Reliability: (4) not assignable
Secondary literature
Reference: Opdyke, D.L.J. 1975 Fragrance raw material monographs - Alcohol C6. 13 (Suppl.) 695-696.

RTECS, 2004.
12-SEP-2004 (46) (55)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: LC50
Species: rat
Strain: Sprague-Dawley
Sex: male/female
No. of Animals: 25
Vehicle: other: air
Doses: 5600 mg/m3
Exposure time: 4 hour(s)
Value: > 5600 mg/m³

Method: other: in house protocol
Year: 1988
GLP: no data
Test substance: > 90% 1-octanol

Remark: Report in Patty of unpublished data from Amoco. No deaths were observed among rats exposed to 6400 mg/m3 (1203 ppm) for 1 hour. 2/10 rats died within 2 hours of a 4 hour exposure to 5600 mg/m3 (1053 ppm). Necrosis of the bronchial epithelium with alveolar oedema and infiltration of alveolar macrophages was observed. No details of the incidence.

Result: MORTALITY: There were no deaths following 1 hour exposure to 6.39 mg/l 1-octanol.

Following 4 hour exposure to 5.6 mg/l. 3/5 male rats died following the 4 hour exposure all females survived:
- Time of death: 1-2 days after exposure.

CLINICAL SIGNS: Salivation and gasping or rapid respiration were observed during and/or immediately after each exposure. Other signs of intoxication included inactivity, rales, coldness, redness around the eys and nose, ocular opacity and exophthalmus and anogenital staining.

BODY WEIGHT: All exposed rats lost body weight following exposure, the survivors of the 4 hour exsoure did not regain weight until day 6 of the exposure period.

NECROPSY FINDINGS: On gross examination treatment related findings were confined to the lungs.

1 hour exposure: lesions described as foci/discoloured areas were observed in 3/5 males and 2/5 females.
4 hour exposure: lesions described as foci/discoloured areas were observed in 4/5 males and 4/5 females. All lungs appeared oedematous.
Controls: 1 male had lung foci.

Histopathological examination of the lungs of rats exposed for one hour revealed no microscopic lesions other than minimal alveolar heamorrhage in 1 male. Lungs from control rats were unremarkable. In animals exposed for 4 hours microscopic lesions included necrosis of the bronchial epithelium (4/5M, 2/5F), alveolar oedema (4/5M, 4/5F) with accumulation of alveolar macrophages (10/10), congestion (2/5M, 1/5F),

alveolar haemorrhage (1/5M, 1/5F), regeneration of the bronchial epithelium (2/5M, 3/5F) and alveolar hyperplasia (1/5F).

POTENTIAL TARGET ORGANS: Lungs

SEX-SPECIFIC DIFFERENCES: Males more susceptible.

Conclusion: The 4 hour rat LC50 for 1-octanol is >5.6 mg/l (nominal). There were clinical signs of respiratory distress and histopathological evidence of irritation of the respiratory tract.

Test condition: TEST ORGANISMS: Rat, SD
- Source: Charles River, Portage, MI, USA
- Age: 6 weeks
- Weight at study initiation: (mean weights) males 340g; females 236g
- Group size: 5M+5F treated
- Controls: 2M+2F untreated

ADMINISTRATION: Inhalation
- Doses: 5.6 mg/l for 4 hours; 6.39 mg/l for 1 hour (nominal conc.) There was no analytical monitoring of the vapour conentration.
- Atmosphere generation: the test substance was heated to approx. 425C and and the resultant vapour administered to the animals in a whole body inhalation chamber.
- Post dose observation period: 7 days

EXAMINATIONS: Clinical observations were made throughout exposure, on removal from the exposure chambers and at least once daily throughout the observation period. Bodyweights of the treated animals were recorded prior to exposure and prior to necropsy. All test and control animals were subject ot gross necropsy and the lungs were examined histopathologically.

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment with restrictions, no measurement of concentration.

Flag: Critical study for SIDS endpoint

Reference: Amoco Corporation, 1988 Acute inhalation toxicity study of capryl alcohol (1-octanol) in rats. Study carried out at IIT Research Institute Study no. 1302A. Submitted to USEPA under TSCA 8(e) December 12th 1988. EPA/OTS Document ID 89-890000051.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols
(Monohydric alcohols) John Wiley & Sons - on line.

RTECS, 2004.
29-DEC-2005 (2) (90) (93)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: LC50
Species: rat
Strain: other: COX-CD
Sex: male/female
No. of Animals: 5
Vehicle: other: atmosphere generated as a mist
Doses: 71 mg/l
Exposure time: 1 hour(s)
Value: > 71 mg/l

Method: other: contract laboratory protocol
Year: 1977
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Result: MORTALITY: All rats survived the 1 hour exposure and subsequent 14 day observation period.

CLINICAL SIGNS: During exposure, all animals displayed hypoactivity and/or ataxia, salivation, and gasping. At the 24 hour period, all animals showed reddened encrustation about the eyes, nose and mouth and a roughened coat. All animals appeared normal within 96 hours following exposure. Final bodyweight records showed weight gains within the expected limits.

NECROPSY FINDINGS: Gross necropsy showed slight to moderate pulmonary congestion in all animals and adrenal congestion in 2 animals.

POTENTIAL TARGET ORGANS: The lungs were affected in all rats.

SEX-SPECIFIC DIFFERENCES:
Source: Scientific Associates, Inc. 1977a
Hayes Consultancy Service Bromley, Kent
Test substance: Tradename Alfol 10
Conclusion: The rat 1 hour LC50 for Alfol 10 (mist) was >71 mg/l. Signs of intoxication during exposure included lethargy,and/or ataxia,

salivation and gasping. Gross necropsy revealed congestion of the lungs in all animals.

Test condition: TEST ORGANISMS: Rat (COX-SD)
- Source: not reported.
- Weight at study initiation: 216-253g
- Number of animals: 5m+5F
- Controls: none

ADMINISTRATION: 1 hour, inhalation, whole body exposure.
- Type of exposure: the atmosphere was generated as a mist, following exposure the animals were washed to remove any accumulated test material.
- Concentrations: 71 mg/l for 1 hour (not monitored)
- Particle size: Droplet size not reported
- Type or preparation of particles: The mist was generated using a nebuliser.
- Postexposure period: 14 days

EXAMINATIONS: The animals were observed frequently on the day of exposure and daily thereafter. Survivors were weighed and necropsied at the end of the exposure period.

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Scientific Associates, Inc. 1977a. Inhalation toxicity test in rats. ALFOL 10 alcohol.
05-AUG-2005 (80)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Type: LC50
Species: mouse
Strain: no data
Sex: no data
Exposure time: 2 hour(s)
Value: = 4 mg/l

Method: other
Year: 1961
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Remark: Secondary report of unobtainable Russian publication also reported in Iuclid 2000 and Patty 2001 (LC50 525 ppm). The only additional data available are confidence limits for the reported LC50 4 mg/l (+- 0.2)
Reliability: (4) not assignable

Secondary reference.
Reference: Ismerov, N.F. et al 1982 Toxicometric parameters of industrial toxic chemicals under single exposure. USSR/UNEP-IRPTC Publication, 1982.

Iuclid 2000 ECB Decanol.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.
08-OCT-2004 (52) (53) (70)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type	:	LC50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Exposure time	:	6 hour(s)
Value	:	> 1.05 mg/l
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	dodecanol (112-53-8)
Remark	:	Test substance dispersed as an aerosol. This is a secondary reference with no experimental detail.
Reliability	:	(4) not assignable Secondary literature
Source	:	Clayton and Clayton 1994 Hayes Consultancy Service Bromley, Kent

Reference Henkel KGaA. 1992. 1-Dodecanol:
03.09.2004 Algen-Zellvermehrungshemmtest. Biological Research and Product safety/Ecology: Unpublished results; Report No. RE 920200.
(7)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Type: other: Inhalation
Species: rat
Strain: other: COX-SD
Sex: male/female
No. of Animals: 5

Vehicle: other: produced as a heated vapour
Doses: 1.5 mg/l
Exposure time: 1 hour(s)
Value: > 1.5 mg/l

Method: other: In house protocol
Year: 1977
GLP: no data
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: MORTALITY: All rats survived the exposure period and subsequent 14 day observation period.

CLINICAL SIGNS: There were no signs of toxicity during the exposure period or the 14 day observation period. All rats gained in bodyweight at an expected rate over the observation period.

NECROPSY FINDINGS: Unremarkable

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None reported.

Source: Scientific Associates, Inc. 1977b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
Conclusion: The rat 1 hour inhalational LC50 for Alfol 14 is >1.5 mg/l. There were no signs of toxicity and findings at gross necropsy were unremarkable.
Test condition: TEST ORGANISMS: Rat (COX-SD)
- Source: not reported.
- Weight at study initiation: 210-299g
- Number of animals: 5M+5F
- Controls: none

ADMINISTRATION: 1 hour, inhalation, whole body exposure.
- Type of exposure: the atmosphere was generated as a heated vapour, following exposure the animals were washed to remove any accumulated test material.
- Concentrations: 1.5 mg/l for 1 hour (not monitored)
- Particle size: vapour
- Type or preparation of particles: The vapour was generated by heating Alfol 14 in a water bath to 60C.
- Postexposure period: 14 days

EXAMINATIONS: The animals were observed frequently on the day of exposure and daily thereafter. Survivors were weighed and necropsied at the end of the exposure period.

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: Scientific Associates, Inc. 1977b. Acute oral toxcity (LD50) in rats, acute dermal toxicity (LD50) in rabbits, dermal irritation test in rabbits, eye irritation test in rabbits, and inhalation toxicity test in rats. ALFOL 14 alcohol.

15-OCT-2004 (64)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)</u>

Type: LC50
Species: rat
Strain: other: Carworth-Wistar
Sex: male/female
No. of Animals: 6
Doses: Saturated vapour concentration
Exposure time: 8 hour(s)

Method: other: Smyth et al, 1962
Year: 1969
GLP: no data
Test substance: other TS: tetradecanol (mixed isomers)

Result: All rats survived this 8 hour static exposure to the concentrated vapours. LC50 > saturated vapour concentration. Result also reported in secondary references Iuclid 2000, Opdyke, 1975, JACT, 1988.

Source: Smyth et al, 1969
Hayes Consultancy Service Bromley, Kent

Test condition: A group of 6 rats (sex unspecified) were exposed to concentrated vapours of the test substance for up to 8 hours using a static exposure technique.

Reliability: (4) not assignable
Screening test only, gives some indication of toxicity but exposure was static, methods described in an earlier publication Smyth et al. Am. In. Hyg. Assoc. J. 23:95-107, 1962.

Reference: Cosmetic Ingredient Review 1988 Final report on the safety assessment of cetearyl alcohol, cetyl alcohol, isostearyl

alcohol, myristyl alcohol and behenyl alcohol. J. Am. Coll. Tox. 7(3): 359-413.

Iuclid 2000 European Commission - European Chemicals Bureau Tetradecanol Cas# 112-72-1.

Opdyke, D.L.J. 1975 Fragrance raw material monographs - Alcohol C14 Myristic. 13(Suppl.) 699-700

Smyth, H.F., Carpenter, C.P., Weil, C.S., Pozzani, U.C., Striegel, J.A., and Nycum, J.S. 1969. Range-finding toxicity data: List VII. Am. Ind. Hyg. Assoc. J. 30(5): 470-476.

01-JAN-2005 (12) (44) (53) (68)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Remark: Secondary report of unpublished data, unobtainable. 10 young Sprague-Dawley rats (average weight 250 g) were exposed (whole body) to an aerosol containing 3% myristyl alcohol. The exposure consisted of intermittent bursts of 10 sec of aerosol, one every 3 minutes, total of 20 in the hour exposure. It was extimated that the average test substance concentration was ca 192 mg/l in air.

None of the exposed animals died. However, following 10 minutes exposure, ataxia and moderate nasal irritation were reported in all test animals persisting throughout the exposure period and for up to 4 hours after removal from the chamber.

Source: JACT, 1988
Hayes Consultancy Service Bromley, Kent

Test substance: Aerosol containing 3% myristyl alcohol (1-hexadecanol).

Reliability: (4) not assignable
Secondary reference.

Reference: Cosmetic Ingredient Review 1988 Final report on the safety assessment of cetearyl alcohol, cetyl alcohol, isostearyl alcohol, myristyl alcohol and behenyl alcohol. J. Am. Coll. Tox. 7(3):359-413

16-JUL-2005 (12)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Remark: Summary report of unpublished data provided by Fassett, originally reported in Patty's 2nd edition, 1963. 6 hour LC50 0.41-2.22 mg/l. All rats died within 2 days at 2.22 mg/l while

all survived at 0.41 mg/l. Concentrations calculated. No further details available. Data is reported in Iuclid 2000 and Opdyke, 1978.

Test substance: hexadecanol. Isomer content and purity not reported.

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Hexadecan-1-ol Cas# 36653-82-4.

Opdyke, D.L.J. 1978 Fragrance raw materials monographs Fd. Cos. Tox. 16: 683-686.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

06-AUG-2005 (50) (66) (67)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Remark: Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C16 (hexadecanol), C16-18, C18 (octadecanol) and C20 (eicosanol) alcohols in support of the statement that C22 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.

Test substance: octadecanol (112-92-5)

Conclusion: The LC50 is expected to be greater than the substantially saturated vapour concentration.

Reliability: (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

Reference: Supporting Robust Summaries: Long Chain Aliphatic Acids Category: 1-Octadecanol.

05-APR-2007

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Type: LC50
Species: rat
Strain: other: Carworth-Wistar
Sex: male/female
No. of Animals: 6
Exposure time: 8 hour(s)

Method: other: Smyth et al, 1962
Year: 1962
GLP: no data
Test substance: other TS: icosanol (mixed isomers)

Result: All rats survived this 8 hour static exposure to the concentrated vapours. LC50 > saturated vapour concentration.
Source: Smyth, 1969
Test condition: A group of 6 rats (sex unspecified) were exposed to concentrated vapours of the test substance for up to 8 hours using a static exposure technique.
Reliability: (4) not assignable
Screening test only, gives some indication of toxicity but exposure was static, methods described in an earlier publication Smyth et al. Am. In. Hyg. Assoc. J. 23:95-107, 1962.

This study is also reported in Patty 2001.
Reference: Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

Smyth, H.F., Carpenter, C.P., Weil, C.S., Pozzani, U.C., Striegel, J.A., and Nycum, J.S. 1969. Range-finding toxicity data: List VII. Am. Ind. Hyg. Assoc. J. 30(5): 470-476.
21-OCT-2004 (17) (19)

<u>1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)</u>

Remark: Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C16 (hexadecanol), C16-18, C18 (octadecanol) and C20 (eicosanol) alcohols in support of the statement that C22 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.
Test substance: >95% 1-docosanol (661-19-8)
Conclusion: The LC50 is expected to be greater than the substantially saturated vapour concentration.
Reliability: (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category.
15-SEP-2005 (26) (29)

5.1.3 Acute Dermal Toxicity

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	LDLo
Value	= 20000 mg/kg bw
Species	Rabbit
Strain	no data
Sex	no data
Number of animals	4
Vehicle	
Doses	no data
Method	other
Year	1968
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Dosage translated from 200 Proof. Reported that dose used killed 1 out of four animals.
Reliability	(4) not assignable No details of method reported therefore not possible to assess compliant with relevant testing protocol. No reference source quoted for reported data.
Reference	Monick, JA (1968) in Alcohols. Their Chemistry Properties and Manufacture. Reinhold 1969, LCCCN 68-23906: p. 75.
12.11.2004	(182)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance:	1-Butanol, Union Carbide sample procured 2/20/48 from Fellowship 155.
Method:	Internal Union Carbide method for dermal toxicity. Thompson's method of calculating the LD50 was used.
Test type:	Acute dermal toxicity (skin penetration).

GLP: No

Year performed: 1951
Species/strain: Rabbit, albino New Zealand, 3-5 months old, 2.5 kg average weight.

Sex: Male
Number of animals/ sex/dose: 4 males/dose x four doses (10.0, 5.0, 2.52, or 1.26 ml/kg).
Vehicle: None
Route of admin.: Undiluted n-butanol was applied for 24 hours to the clipped trunks of the rabbits.
Results: Dermal LD50 = 4.2 (3.0 to 6.0) ml/kg. = 3.402 g/kg = 3402 mg/kg

Mortality at 10.0ml/kg = 4/4
Mortality at 5.0 ml/kg 3/4
Mortality at 2.52 ml/kg = 0/4
Mortality at 1.26 ml/kg 0/4
Comments: Observation period was 14 days. All mortality occurred on day 0.
Data quality: Reliability: Key study. Klimisch quality 2.
References: Union Carbide Corp. Bushy Run Research Center, Project Report No.14-73. Export, PA. 1951.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species/strain: Rabbit
Test method: Not Stated
GLP: No

Test results: LD50 5.3 g/kg
Comments:
Reference: Patty, F.A. 1982. Industrial Hygiene and Toxicology, 3rd ed., New York, Chichester, Brisbane, Toronto, Singapore, WileyInterscience. IIC: 4571-4578. As cited in World Health Organization (WHO). 1987. Environmental Health Criteria 65:
Butanols - Four Isomers: 1-Butanol, 2-Butanol, tert-Butanol, Isobutanol. WHO.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species/strain: Rabbit
Test method: Not Stated
GLP: No

Test results: LD100 7.5 g/kg
Comments:
Reference: Patty, F.A. 1982. Industrial Hygiene and Toxicology, 3rd ed., New York, Chichester, Brisbane, Toronto, Singapore, WileyInterscience. lIC: 4571-4578. As cited in World Health Organization (WHO). 1987. Environmental Health Criteria 65:
Butanols Four Isomers: 1-Butanol 2-Butanol tert-Butanol Isobutanol. WHO.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LD50
Species: rat
Strain: New Zealand white
Sex: male/female
No. of Animals: 40
Vehicle: other: applied undiluted
Doses: 1, 2, 3 and 4 g/kg
Value: = 2330 mg/kg bw

Method: other: contract laboratory protocol
Year: 1980
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: MORTALITY:
- Time of death: Deaths occurred from day one until day 10 of the observation period for both intact and abraded skin.
- Number of deaths at each dose: 0/10, 3/10, 5/10, 10/10 combined male and female mortality for intact skin. 0/10, 4/10, 8/10, 10/10 combined male and female mortality for abraded skin.

LD50(s): Intact skin M+F 2.33 g/kg (1.81-2.99) Males 2.40 g/kg (1.66-3.48) Females 2.39 g/kg (1.60-3.56). Abraded skin M+F 2.15 g/kg (1.71-2.71) Males 2.15 g/kg (1.55-2.00) Females 2.15 g/kg (1.55-2.99) Combined intact and abraded M+F 2.24 g/kg.

APPLICATION SITE: Slight to severe erythema in most animals at all dose levels, slight to servere oedema in all animals at all dose levels. At 24 hours thickening, blanching and wrinkling was also reported. Erythema and oedema persisted to 72 hours in some animals. At days 7 and 14 these changes progressed to thickening , maceration, wrinkling, dryness, coriaceousness, desquamation, sloughing and scar tissue

formation.

CLINICAL SIGNS: These were reported combined for intact and abraded skin and males and females.
1 g/kg: 2/20 animals appeared thin by observation day 7. An overall weight loss was reported for 4/20 rats (1 intact skin) ranging from 0.42 (intact) to 17.36% (abraded).
2 g/kg: 15/20 showed some of the following- pallor, hypersensitivity to touch, generalised weakness, malaise, hunched position and thinness. 7/13 survivors showed a weight loss.
3g/kg: 17/20 showed some of the following: pallor, generalised weakness, hunched position, diarrhoea, hypothermia, dyspnea, thinness, prostration, moribundity. All survivors showed either weight loss or minimal weight gain.
4 g/kg: 7/20 surivived more than 24 hours and these showed some of the following prior to death: pallor, hypersensitivity to touch, generalised weakness, hypothermia, prostration. All animals died by observation day 5.

NECROPSY FINDINGS: 1g/kg: All animals survived to the end of the observation period in 14/20 necropsy finding were unremarkable. Two animals showed accumulation of clear fluid in the peritoneal cavity, 3 pale-tan kidneys, and 3 a decrease in fatty tissue in the viscera.

2g/kg: 13 animals survived, of these necropsy findings were unremarkable in 7 rabbits. Two surviving animals had accumulation of clear fluid in the peritonal cavity, 1 severe erosion of the gastric mucosa, and 5 depletion of visceral fat. Among the 7 mortalites, 1 showed a slight accumulation of clear fluid in the peritoneal cavity, 3 severe congestion of the kidneys, 6 erosion of the gastric mucosa, 1 congestion of the lungs, 2 a friable liver, 4 depletion of visceral fat, and one post mortem autolysis of visceral organs.

3g/kg: 7 animals survived of these necropsy findings were unremarkable in 4 rabbits. In other surviving animals 1 animal with pale-tan kidneys, 1 with enlarged kidneys, 1 with a thickened stomach wall, and 1 with depletion of visceral fat. In the animals which died, 3 animals had congestion of the kidneys, 12 severe erosion of the gastric mucosa, 2 congestion of the lungs, 2 a mottled liver, 5 congestion of the small intestines, 1 congestion of the caecum, 1 reddish tinged urine , and 2 with post-mortem autolysis of the abdominal viscera.

4 g/kg: All animals died. Five animals showed congestion of the kidneys, 12 severe erosion of the gastric mucosa, 5 congestion of the lungs, 1 accumulation of fluid in thoracic

cavity, 4 reddish tinged urine, and 2 post-mortem autolysis of the abdominal viscera. In one animal findings were unremarkable.

POTENTIAL TARGET ORGANS: gastric mucosa

SEX-SPECIFIC DIFFERENCES: No marked difference in LD50. Clinical signs were not reported separately.

Source: Scientific Associates, Inc. 1980
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rabbit (New Zealand White)
- Source: not reported
- Age: not reported
- Weight at study initiation: 2.3 - 3.02 kg
- Group size: 5M+5F
- Controls: none

ADMINISTRATION: 24 hour application to intact and abraded skin
- Area covered: the dose was applied to the trunk of the animals under occlusion.
- Occlusion: plastic binder
- Vehicle: Applied undiluted.
- Total volume applied: maximum dose 3-4 ml/kg
- Doses: 1, 2, 3 and 4 g/kg
- Removal of test substance: Excess material removed with absobent paper towels. Attempts were made to estimate the amount of unabsorbed material but this was not possible.

EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation days 7 and 14. All decedents and survivors were subject to gross necropsy. The LD50 was calculated using the method of Litchfield and Wilcoxon, 1949.

Test substance: Tradename Alfol 6

Conclusion: The rabbit dermal LD50 for Alfol 6 following a 24 occluded exposure to intact skn is 2.33 g/kg. There was significant evidence of skin irritation at the application site persisting in some animals throughout the observation period. Clinical signs were indicative of a general toxic effect coupled with anorexia. The most common gross pathological finding was

erosion of the gastric mucosa.
Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restirictions.
Well documented and well conducted study not to GLP.
Flag: Critical study for SIDS endpoint
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3

Scientific Associates, Inc. 1980. Acute dermal toxicity (LD50) test in rabbits (Alfol 6 Alcohol).
15-JUL-2005 (29) (63)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LD50
Species: rabbit
Strain: New Zealand white
Sex: male/female
No. of Animals: 16
Vehicle: other: undiluted
Doses: 0.5, 1, 1.5 and 2 g/kg
Value: = 1500 - 2000 mg/kg bw

Method: other: contract laboratory protocol
Year: 1977
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: MORTALITY:
- Time of death: Within 48 hours of dosing.
- Number of deaths at each dose: 0/4, 1F/4, 1M/4, 4/4.

Rabbit dermal LD50 (24 hour occlusive exposure) 1.5 - 2 g/kg. This is a combined value for intact and abraded skin and males/females.

APPLICATION SITE: At 24 hours all animals showed slight to moderate erythema especially of the ventral region. Survivors all showed wrinkling and/or coriaceousness, hardening and desquamation of the skin which persisted throughout the observation period.

CLINICAL SIGNS: Prior to death generalised weakness and/or unthriftiness, diarrhoea, hypothermia, pallor, loss of corneal and palepebral reflexes, hunched position, flaccidity, slow shallow repsiration and coma. Similar signs of intoxication

but less marked were observed in survivors. All survivors appeared systemically normal within 96 hours of dosing. Among survivors there was weight loss in 3 rabbits, one rabbit maintained a constant weight, while the remaining survivors showed weight gains within expected limits.

NECROPSY FINDINGS: Premature decedents showed at gross necropsy, in addition to dermal irritation, severe haemorrhaging and/or bloody, gelatinous infiltration of the subcutis, depletion of fatty tissue, slight accumulation of clear fluid within the peritoneal cavity, moderate congestion of liver and kidneys and severe haemorrhaging and/or blanching of the gastric mucosa.

Amongst survivors (10), other than residual skin damage, gross necropsy findings were unremarkable in 7 rabbits. In the remaining 3 rabbits there was a slight to moderate accumulation of clear viscous liquid in the peritoneal cavity and/or a dpeletion of visceral fat and mottling or stippling of the renal cortex.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None obvious.

Source: Scientific Associates, Inc. 1977c
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rabbit (New Zealand White)
- Source: Not reported.
- Age: Not reported.
- Weight at study initiation: 2.3 - 2.9 kg
- Group size: 2M+2F intact and abraded skin
- Controls: None

ADMINISTRATION: 24 hour occlusive
- Area covered: Not reported.
- Occlusion: Plastic binder.
- Vehicle: Undiluted
- Doses: 0.5, 1, 1.5 and 2 g/kg
- Removal of test substance: Washing and blotting dry with paper towels.

EXAMINATIONS: The animals were observed for clinical signs of intoxication several time during the day of dosing and daily thereafter throughout the 14 day observation period. The animals were weighed at sacrifice. All premature decedents and survivors were subjected to gross necropsy.

Test substance: Tradename Alfol 6
Conclusion: The rabbit dermal 24 hour occlusive LD50 (combined applications to intact and abraded skin) is 1500-2000 mg/kg.
Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions (small group size).
Flag: Critical study for SIDS endpoint
Reference: Associates, Inc. 1977c. Acute oral toxicity (LD50) in rats; Acute dermal toxicity (LD50) in rabbits, Dermal irritation test in rabbits; Eye irritation test in rabbits; Inhalation toxicity tests in rats: ALFOL 6. S.A. Number 233619.

Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3
11-NOV-2004 (7) (29)

<u>1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)</u>

Type: LD50
Species: rabbit
Vehicle: other: undiluted
Value: = 3100 ml/kg bw

Method: other: Draize, 1944
Year: 1951
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Result: The acute dermal LD50 for n-hexanol is reported as 3100 ml/kg (confidence limits 2020-4770) equivalent to 2530 mg/kg.
Test condition: The dermal toxicity of n-hexanol in the rabbit was determined using a modification of the rubber cuff method advocated by the FDA at the time of this study. The test material was applied undiluted and remained in contact with the skin under an occlusive dressing for 24 hours. Animals were then observed for 14 days and mortality recorded. No further details of group size, clinical signs etc were available.
Reliability: (4) not assignable
Documentation insufficient for assessment.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

RTECS, 2004

Smyth, H.F., Carpenter, C.P., and Weil, C.S. 1951.
Range-finding toxicity data: List IV. A.M.A. Archives of
Industrial Hygiene and Occupational Medicine 4: 119-122.
13-OCT-2004 (29) (48) (55) (68)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: LD50
Value: > 5000 mg/kg bw

Method: other
Year: 1975
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Remark: The acute dermal LD50 in rabbits is reported as >5000 mg/kg.
Reliability: (4) not assignable
Secondary reference no experimental details given.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau
hexan-1-ol Cas# 111-27-3.

Opdyke, D.L.J. 1975 Fragrance raw material monographs -
Alcohol C6. 13(Suppl.) 695-696.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols
(Monohydric alcohols) John Wiley & Sons - on line.
12-SEP-2004 (29) (46) (48)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Remark: Other LD50 values are reported in IUCLID 2000 ascribed to
either Henkel (1) or the Dangerous Properties of Industrial
Materials Report for hexanol (2).

The values are for rabbits and are as follows:

LD50 2530 mg/kg (1)
LD50 2500 mg/kg (2)

No experimental details are given.
Reliability: (4) not assignable
Secondary references.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau
hexan-1-ol Cas# 111-27-3

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: LD50
Species: rabbit
Strain: New Zealand white
Sex: male/female
No. of Animals: 16
Vehicle: other: undiluted test substance
Doses: 1, 2 and 4 g/kg
Value: = 2000 - 4000 mg/kg bw

Method: other: contract laboratory protocol
Year: 1976
GLP: no data
Test substance: > 90% 1-octanol

Result: MORTALITY:
- Time of death: All deaths occurred within 4 days of exposure.
- Number of deaths at each dose: Intact skin 0/2, 1/4 and 2/2, abraded skin 0/2, 3/4 and 2/2.

LD50(s): Intact skin: 2-4 g/kg; Abraded skin: 1-2 g/kg; combined intact and abraded 2 g/kg. A visual assessment of test site suggested that >75% of the dose was observed at each dose level.

APPLICATION SITE: At the end of the exposure period all animals showed slight to severe erythema and oedema particulary of the ventral skin and particularly in animals with abraded skin. In all survivors wrinkling and coreaceousness gradually developed forming and inelastic sheath around the trunk of the animal. The healing process continued throughout the 14 day observation period.

CLINICAL SIGNS: Generalised weakness and inactivity in most animals following exposure. Survivors appeared normal at 72 hours post exposure. These signs persisted and/or intensified in animals which eventually died. Final body weights of surviving animals showed moderate to severe loss in 2 animals, constant weight in 3 animals, and slight to moderate gain in 3 animals.

NECROPSY FINDINGS: In animals which succumbed there was severe

skin damage with maceration and erosion of the ventral skin and musculature. Blanching and multiple focal haemorrhages of the gastric mucosa, friability of the liver, moderate heamaturia and a slight accumulation of amber, watery

peritoneal fluid were observed internally.

Rabbits surviving to 14 days showed moderate to marked desquamation, severe erosion and multiple focal haemorrhages of the gastric mucosa and slight accumulation of clear or amber viscous fluid in the peritoneal cavity.

POTENTIAL TARGET ORGANS: Gastric mucosa.

SEX-SPECIFIC DIFFERENCES: The experimental data was reported in combined form.

Source: Scientific Associates, Inc. 1976a
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rabbit (New Zealand White)
- Source: not reported
- Age: not reported
- Weight at study initiation: 2.3 - 2.9 kg
- Group size: low dose and high dose 2M+2F and mid dose 4M+4F half with intact skin the others with abraded skin.
- Controls: none

ADMINISTRATION: 24 hour application to intact and abraded skin
- Area covered: the dose was applied to the trunk of the animals under occlusion.
- Occlusion: plastic binder
- Vehicle: Applied undiluted.
- Total volume applied: maximum dose 3-4 ml/kg
- Doses: 1, 2 and 4 g/kg
- Removal of test substance: Excess material removed with absorbent paper towels. An estimate was made of the the amount of unabsorbed material.

EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation day 14. All decedents and survivors were subject to gross necropsy.

Conclusion: The rabbit dermal LD50 for Alfol 8 following 24 hour occlusive exposure was 2000-4000 mg/kg. There was significant evidence of skin irritation at the application site persisting in some

animals throughout the observation period. Clinical signs were indicative of a general toxic effect coupled with anorexia. The most common gross pathogical finding was erosion of the gastric mucosa.

Reliability: (2) valid with restrictions
Study reasonably well conducted and reported. Particularly where the skin was abraded the degree of irritation reported at the contact site (full depth erosion) may have contributed to the death of the animals.

Flag: Critical study for SIDS endpoint

Reference: Scientific Associates, Inc. 1976a. Acute dermal toxicity (LD50) in rabbits. ALFOL 8 alcohol.

14-SEP-2004 (101)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: LD50
Species: rabbit
Value: > 5000 mg/kg bw

Year: 1972
Test substance: > 90% 1-octanol (111-87-5)

Remark: Secondary report of unpublished data from Levenstein, 1972 report to RIFM.

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Octan-1-ol Cas# 111-87-5

Opdyke, D.L.J. 1973 Monographs on fragrance raw materials. Fd. Cos. Tox. 11:95-115.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

RTECS, 2004

14-SEP-2004 (62) (88) (90) (93)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: LD50
Species: guinea pig
Value: > 500 mg/kg bw

Year: 1972

Test substance: other TS: 2-octanol

Remark: This value is reported in several secondary references as being the LD50 value for n-octanol. These sources are erroneous, the original report in Patty 1963 of an unpublished reference by Fassett is clearly a value for 2-octanol. This value does not appear in Patty 2001.

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Octan-1-ol Cas# 111-87-5.

Opdyke, D.L.J. 1973 Monographs on fragrance raw materials. Fd. Cos. Tox. 11:95-115.

RTECS, 2004.

14-SEP-2004 (62) (88) (93)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: LD50
Species: rabbit
Strain: New Zealand white
Sex: male/female
No. of Animals: 16
Vehicle: other: Undiluted alcohol spread over skin
Doses: 1, 2 and 4 g/kg
Value: = 2000 - 4000 mg/kg bw

Method: other: contract laboratory protocol
Year: 1976
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Result: MORTALITY:
- Time of death: All deaths occurred within 3 days of exposure.
- Number of deaths at each dose: Intact skin 0/2, 0/4 and 2/2, abraded skin 0/2, 2/4 and 2/2.

LD50(s): Intact skin: 2-4 g/kg; Abraded skin: 2 g/kg; combined intact and abraded 2-4 g/kg. A visual assessment of test site suggested that >75% of the dose was absorbed at each dose level.

APPLICATION SITE: At the end of the exposure period all

animals showed slight to moderate erythema and slight to marked oedema particularly of the ventral skin and particularly in animals with abraded skin. In all survivors, slight to severe drying and desquamation, wrinkling and coreaceousness of limited areas an multiple scattered pustular eruptions later occured persisting throughout the 14 day observation period.

CLINICAL SIGNS: Generalised weakness and inactivity in most animals following exposure. Survivors appeared normal at 72 hours post exposure. These signs persisted and/or intensified in animals which eventually died. Final body weights of surviving animals showed slight to moderate loss loss in 3 animals, remained constant in 1 animal, and showed slight to moderate gain in 6 animals.

NECROPSY FINDINGS: Dermal irritation as described above. Blanching, erosion and multiple focal haemorrhages of the gastric mucosa, haematuria and an accumulation of clear, viscous fluid within the peritoneal cavity were observed internally in animals which died prematurely.

Rabbits surviving to 14 days all showed moderate to severe desquamation with multiple interspersed scars at the application site (some 2-3 cm in diameter). Internally there was a slight accumulation of clear viscous fluid in the peritoneal cavity. There was blanching and/or focal haemorrhages and a granular texture to the gastric mucosa.

POTENTIAL TARGET ORGANS: Gastric mucosa.

SEX-SPECIFIC DIFFERENCES: The experimental data was reported in combined form.

Source: Scientific Associates, Inc. 1976b
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rabbit (New Zealand White)
- Source: not reported
- Age: not reported
- Weight at study initiation: 2.4 - 2.9 kg
- Group size: low dose and high dose 2M+2F and mid dose 4M+4F half with intact skin the others with abraded skin.
- Controls: none

ADMINISTRATION: 24 hour application to intact and abraded skin
- Area covered: the dose was applied to the trunk of the animals under occlusion.

- Occlusion: plastic binder
- Vehicle: Applied undiluted.
- Total volume applied: maximum dose 3-4 ml/kg
- Doses: 1, 2 and 4 g/kg
- Removal of test substance: Excess material was washed away and the area dried with absorbent paper towels. An estimate was made of the the amount of unabsorbed material.

EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation day 14. All decedents and survivors were subject to gross necropsy.

Test substance: Tradename Alfol 10

Conclusion: The rabbit dermal LD50 for Alfol 10 was between 2000 and 4000 mg/kg (24 hour occlusive exposure). Dermal irritation was observed at the application site 24 hours after administration of the test material and persisted throughout the observation period. Generalised weakness and inactivity were commonly observed following the exposure period. Necropsy revealed blanching, erosion and focal haemorrhages in the gastric mucosa.

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: Scientific Associates, Inc. 1976b. Acute dermal toxicity (LD50) in rabbits. Alfol 10 alcohol.

05-AUG-2005 (79)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Type: LD50
Species: rabbit
Strain: New Zealand white
Sex: male
No. of Animals: 6
Vehicle: other:
Doses: 1000 mg/kg
Value: > 1000 mg/kg bw

Method: other: in house protocol
Year: 1979
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Result: MORTALITY: All animals survived the exposure period and 14 day observation period.

CLINICAL SIGNS: Confined to slight irritation of the skin reversible in 7 days. No signs of systemic toxicity.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified other than slight skin irritaton.

SEX-SPECIFIC DIFFERENCES: Males only tested.

Source: Potokar, 1979
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rabbit (New Zealand White)
- Source: Not reported
- Weight at study initiation: Not reported
- Group size: 6M
- Controls: No

ADMINISTRATION: 24 hour dermal occluded.
- Area covered: 10cm X 10cm
- Occlusion: gauze attached with plaster covered with plastic foil and then with elastic bandage.
- Vehicle: undiluted
- Doses: 1000 mg/kg
- Removal of test substance: Not reported.

EXAMINATIONS: 14 day observation period for mortality, signs of intoxication and local skin reaction.

Test substance: Tradename Lorol 10.

Conclusion: The rabbit dermal LD50 for Lorol C10 is >1000 mg/kg (24 hour occluded exposure). There were no signs of systemic toxicity only slight reversible skin irritation.

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: Potokar, 1979. Lorol 810 und Lorol C 10, toxikologische Untersuchungen. No. 281. 27 November 1979.

08-OCT-2004 (71)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Type: LD50

Species: rabbit
Value: = 18.8 ml/kg bw

Method: other
Year: 1972
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Remark: Secondary report of unobtainable Russian publication also reported in Iuclid 2000. No other information available.
Reliability: (4) not assignable
Secondary reference.
Reference: Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.
08-OCT-2004 (70)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type	:	LD50
Value	:	= 8000 - 12000 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	4
Vehicle	:	other: undiluted
Doses	:	0.5, 1, 2, 4, 6, 8 and 12 g/kg
Method	:	other: contract laboratory protocol
Year	:	1977
GLP	:	no
Test substance	:	dodecanol (112-53-8)
Test substance	:	Tradename Alfol 12
Test condition	:	TEST ORGANISMS: Rabbit (New Zealand White) - Source: not reported - Age: not reported - Weight at study initiation: 2.28 - 3.04 kg - Group size: low dose and high dose 2M+2F - Controls: none ADMINISTRATION: 24 hour application to intact and abraded skin - Area covered: the dose was applied to the trunk of the animals under occlusion. - Occlusion: plastic binder - Vehicle: Applied undiluted.

- Total volume applied: maximum dose 11-12 ml/kg
- Doses: 0.5, 1, 2, 4, 8 and 12 g/kg
- Removal of test substance: Excess material was washed away and the area dried with absorbent paper towels. An estimate was made of the the amount of unabsorbed material.

EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation day 14. All decedents and survivors were subject to gross necropsy.

Result : MORTALITY:
- Time of death: All deaths occurred between days 2 and 10 after administration.
- Number of deaths at each dose: Intact skin 0/2, 0/2, 2/2, 1/2, 1/2, abraded skin 0/2, 1/2, 0/2,0/2, 1/2, 1/2. Combined 0/4, 1/4, 2/4, 1/4, 2/4, 2/4. It appeared that most of the test substance was absorbed.

LD50(s): The LD50 for combined abraded and intact skin was considered to be between 8 and 12 g/kg. The small group size and erratic dose response precluded separate estimation for intact and abraded skin.

APPLICATION SITE: At the end of the exposure period all animals showed slight to moderate erythema at the application site. In all survivors wrinkling and/or coreaceousness, hardening and desquamation of the skin occurred and persisted in varying degrees until the end of the observation period.

CLINICAL SIGNS: Generalised weakness and/or unthriftiness preceded death in each animal. Similar effects but to a lesser degree were observed in some survivors. 11/16 survivors appeared normal witin 96 dose of exposure. Final body weights of surviving animals showed slight to moderate loss in 8 animals, constant weight in 2 animals, and gains within expected limits in 6 animals.

NECROPSY FINDINGS: Animals which died showed one or more of the following: depletion of visceral fatty tissue, moderate accumulation of clear fluid within the peritoneal cavity, moderate congestion of lungs and kidneys, haemorrhaging and/or blanching with erosion of the gastric mucosa.

Rabbits surviving to 14 days showed slight to moderate accumulation of clearr viscous liquid within the peritoneal cavity and/or depletion of visceral fatty tissues. 9/16 rabbits showed no gross systemic

changes.

POTENTIAL TARGET ORGANS: Gastric mucosa.

SEX-SPECIFIC DIFFERENCES: More females than males succumbed to the effects of the test material.

Conclusion : The rat dermal LD50 for this sample of Alfol 12 was in the range of 8000-12000 mg/kg (24 occluded exposure). All test animals developed skin irritation at the application site persisting throughout the observation period. Clinical signs of toxicity were generalised weakness and unthriftiness. Haemorrhage and/or blanching with erosion of the gastric mucosa was reported in premature decedents but not in rabbits which survived to the end of the exposure period.

Reliability : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Source : Scientific Associates, Inc. 1977f
Hayes Consultancy Service Bromley, Kent.

Flag : Critical study for SIDS endpoint

Reference Veith, G.D., Call, D.J., and Brooke, L.T. 1983b. Structure-toxicity relationships for the fathead minnow, Pimephales promelas: Narcotic industrial chemicals. Can. J. Fish. Aquat. Sci. 40:743-748.

11.08.2005 (24)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type : LD50
Value : = 1500 - 2000 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 4
Vehicle : other: applied undiluted
Doses : 1, 1.5 and 2 g/kg
Method : other: contract laboratory protocol
Year : 1975
GLP : no
Test substance : dodecanol (112-53-8)

Test substance : Tradename Alfol 12

Test condition : TEST ORGANISMS: Rabbit (New Zealand White)
- Source: not reported
- Age: not reported
- Weight at study initiation: 2.2 - 3.1 kg
- Group size: 2M+2F
- Controls: none

ADMINISTRATION: 24 hour application to intact and abraded skin
- Area covered: the dose was applied to the trunk of the animals under occlusion.
- Occlusion: plastic binder
- Vehicle: Applied undiluted.
- Total volume applied: maximum dose 1-2 ml/kg
- Doses: 1, 1.5 and 2 g/kg
- Removal of test substance: Excess material was washed away and the area dried with absorbent paper towels.

EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation day 14. All decedents and survivors were subject to gross necropsy.

Result : MORTALITY:
- Time of death: All deaths occurred within 3 days of exposure.
- Number of deaths at each dose: Intact skin 0/2, 1/2 and 2/2, abraded skin 0/2, 0/2 and 2/2.

LD50(s): Intact skin: 1.5 g/kg; Abraded skin: 1.5 - 2 g/kg; combined intact and abraded 1.5 - 2 g/kg. At the end of the 24 hour exposure period it appeared that some absorption of test material had occurred.

APPLICATION SITE: Animals at all dose levels showed erythema, wrinkling and desquamation of the application site.

CLINICAL SIGNS: At ta dose of 1g/kg there were no signs of toxicity. At higher dose levels some prostration was noted. Survivors appeared normal 72 hours after exposure. Survivors generally gained weight within expected limits with 2 exceptions one intact male at 1 g/lg sowed a slight weight loss and one abraded male at 1.5 showed a constant weight.

NECROPSY FINDINGS: In premature decedents there was some general deterioration but no dose-related lesions. Tissues of survivors sacrificed at the end of the observation period were unremarkable.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: The experimental data was reported in combined form.

Conclusion : The rabbit dermal LD50 of Alfol 12 was between 1500 and 2000 mg/kg. All rabbits showed irritation of the application site immediately following exposure. Some prostration was observed in animals at the higher dose levels. Necropsy findings showed no treatment related lesions.

Reliability : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Source : Scientific Associates, Inc. 1975
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Veith, G.D., Call, D.J., and Brooke, L.T. 1983a. Estimating the acute toxicity of narcotic chemicals to fathead minnows. In: Bishop, W.E., Cardwell, R.D., and Heidolph, B.B. (eds.). Aquatic Toxicology and Hazard Assessment: Sixth Symposium. ASTM STP 802. American Society for Testing and Materials, Philadelphia.

11.08.2005 (23)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type : LD50
Value : > 8310 mg/kg bw
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: not specified
Year :
GLP : no data
Test substance : other TS: Dodecanol (112-53-8)

Remark : Secondary reference, limited data this was a personal communication provided by Fassett for the 1963 edition of Patty.

Reliability : (2) valid with restrictions

Source : Clayton and Clayton 1994
Hayes Consultancy Service Bromley, Kent

Reference Hattori, M., (1987), Effects of long-chain fatty acids and fatty alcohols on the growth of Streptococcus mutans, Chem. Pharm. Bull. 35:3507-3510.

03.09.2004 (6)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Type: LD50
Species: rabbit
Strain: New Zealand white
Sex: male/female
No. of Animals: 4
Vehicle: other: 50% w/w dilution tetradecanol in 1 % w/w gum tragacanth
Doses: 2, 4 and 8 g/kg
Value: = 8000 mg/kg bw

Method: other: Contract laboratory protocol
Year: 1977
GLP: no data
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: MORTALITY:
- Time of death: On observation days 9 and 11.
- Number of deaths at each dose: abraded 0/2, 0/2 and 2/2; intact 0/2, 0/2, 0/2.

LD50 M+F 8000 mg/kg It appeared that most of the test material remained unabsorbed on the skin.
APPLICATION SITE: At 24 hours after administration all animals showed slight to moderate erythema, desquamation, wrinkling and dryness. In all surviving animals desquamation and wrinkling persisted to the end of the observation period.

CLINICAL SIGNS: At 8000 mg/kg, two surviving animals showed signs of weakness, emaciation and pallor. All returned to normal within 4 days of exposure. Body weights of surviving animals showed a slight loss in 1 animal, constant weight in 1 animal and gains within expected limits in 8 animals.

NECROPSY FINDINGS: Animals which succumbed showed depleted visceral fatty tissue (1 rabbit), moderate dermal irritation, and desquamation at the treatment site (2 rabbits). One

animal, which was sacrificed, showed a slight accumulation of clear, viscous fluid within the peritoneal cavity and crazing over the kidney cortex. In all other animals the necropsy findings were unremarkable.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.

Source: Scientific Associates, Inc. 1977b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS: Rabbit (New Zealand White)
- Source: not reported
- Age: not reported
- Weight at study initiation: 2.3-2.9 kg
- Group size: 2M+2F (1M+1F each intact and abraded)
- Controls: none

ADMINISTRATION: 24 hour application to intact and abraded skin
- Area covered: the dose was applied to the trunk of the animals under occlusion.
- Occlusion: plastic binder
- Vehicle: 50% in 1% w/w gum tragacanth
- Total volume applied: maximum dose 3-4 ml/kg
- Doses: 2, 4 and 8 g/kg
- Removal of test substance: Excess material was washed away and the area dried with absorbent paper towels. An estimate was made of the amount of unabsorbed material.

EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation day 14. All decedents and survivors were subject to gross necropsy.

Test substance: Tradename Alfol 14

Conclusion: The rabbit dermal LD50 (24 hour occluded) for Alfol 14 was approx. 8000 mg/kg. All survivors showed skin irritation at the application site throughout the observation period. Signs of intoxication included weakness, emaciation and pallor.

Reliability: (2) valid with restrictions

Flag: Critical study for SIDS endpoint

Reference: Scientific Associates, Inc. 1977b. Acute oral toxcity (LD50) in rats, acute dermal toxicity (LD50) in rabbits, dermal irritation test in rabbits, eye irritation test in

rabbits, and inhalation toxicity test in rats. ALFOL 14 alcohol.
16-JUL-2005 (64)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Type: LD50
Species: rabbit
Strain: New Zealand white
Sex: male
Vehicle: other: undiluted
Value: = 7.13 ml/kg bw

Method: other: Smyth et al, 1962
Year: 1969
GLP: no data
Test substance: other TS: tetradecanol (mixed isomers)

Result: Results were not reported in detail. The LC50 was 7.13 ml/kg (confidence limits 4.41-11.52 ml/kg). Equivalent to 5847 mg/kg using the density of 0.82 g/cm3, reported in chapter 2.3. No other details available.
Source: Smyth 1969
Hayes Consultancy Service Bromley, Kent
Test condition: TEST ORGANISMS: rabbit
- Source: no data
- Weight at study initiation: 2.5 -3.5 kg
- Group size: 4
- Controls: no

ADMINISTRATION: dermal
- Area covered: entire trunk
- Occlusion: Yes
- Vehicle: none
- Concentration in vehicle: undiluted

EXAMINATIONS: Clinical signs, 14 day observation period.
Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment. Study considered valid although result reporting is limited.
Reference: Smyth, H.F., Carpenter, C.P., Weil, C.S., Pozzani, U.C., Striegel, J.A., and Nycum, J.S. 1969. Range-finding toxicity data: List VII. Am. Ind. Hyg. Assoc. J. 30(5):470-476.
11-MAY-2006 (68)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Remark: Secondary report of unpublished data provided by Levenstein, 1974 (original unobtainable). The acute dermal LD50 in rabbits is reported as >5g/kg. This values also reported by RTECS, 2004, Iuclid 2000 and Patty 2001.
Source: Opdyke, 1975
Hayes Consultancy Service Bromley, Kent
Test substance: > 95% 1-Tetradecanol (112-72-1)
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau Tetradecanol Cas# 112-72-1.

Opdyke, D.L.J. 1975 Fragrance raw material monographs - Alcohol C14 Myristic. 13(Suppl.) 699-700.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

RTECS, 2004.
16-OCT-2004 (44) (53) (54) (57)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Test substance: 1-hexadecanol (36653-82-4)
Remark: Report of unpublished data. Rabbit LD50 >5000 mg/kg. No further details available. Study reported in Iuclid 2000.
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau Hexadecan-1-ol Cas# 36653-82-4.

Opdyke, D.L.J. 1978 Fragrance raw materials monographs Fd. Cos. Tox. 16: 683-686.
18-OCT-2004 (50) (66)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Remark: Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-20). This includes data reported for C16-18 alcohols and C20 (1-eicosanol) alcohols. This data supports the statement that C18 alcohols are expected to be of low acute dermal toxicity LD50 >2000 mg/kg.

Test substance: octadecanol (112-92-5)
Conclusion: Expected to be of low toxicity LD50 >2000 mg/kg
Reliability: (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
Reference: SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.
05-APR-2007

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Type: LD50
Species: rabbit
Strain: New Zealand white
Sex: male
No. of Animals: 4
Value: > 20 ml/kg bw

Method: other: Smyth et al, 1962
Year: 1962
GLP: no data
Test substance: other TS: icosanol (mixed isomers)

Result: Results were not reported in detail. The LD50 was >20 ml/kg. (>16,800 mg/kg using the density of 0.84 g/cm3 reported in chapter 2.3). No further details available.
Source: Smyth, 1969
Test substance: TEST ORGANISMS: rabbit
- Source: no data
- Weight at study initiation: 2.5 -3.5 kg
- Group size: 4
- Controls: no

ADMINISTRATION: dermal
- Area covered: entire trunk
- Occlusion: Yes
- Vehicle: none
- Concentration in vehicle: undiluted

EXAMINATIONS: Clinical signs, 14 day observation period.
Reliability: (2) valid with restrictions
Meets generally accepted scientific principles, acceptable for assessment. Study considered valid although result reporting is limited.
Reference: Smyth, H.F., Carpenter, C.P., Weil, C.S., Pozzani, U.C.,

Striegel, J.A., and Nycum, J.S. 1969. Range-finding toxicity data: List VII. Am. Ind. Hyg. Assoc. J. 30(5):470-476.

11-MAY-2006 (19)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Remark: Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-20). This includes data reported for C16-18 alcohols and C20 (1-eicosanol) alcohols. This data supports the statement that C22 alcohols are expected to be of low acute dermal toxicity LD50 >2000 mg/kg.
Test substance: >95% 1-docosanol (661-19-8)
Conclusion: Expected to be of low toxicity LD50 >2000 mg/kg
Reliability: (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
Reference: SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category
15-SEP-2005 (26) (29)

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Test substance: 1-triacontanol (593-50-0)
Remark: Rabbit LD50 >2000 mg/kg bw. No further details available.
Reliability: (4) not assignable
Reference: EPA (1983). US Environmental Protection Agency. Tolerances and Exemptions from Tolerances for Pesticide Chemical in or on Raw Agricultural Commodities: 1-Triacontanol. Fed. Reg. 48, (92), 21132.
05-APR-2007

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rabbit
Concentration	Undiluted
Exposure	Occlusive
Exposure time	4 hour(s)
Number of animals	6
Vehicle	
PDll	
Result	not irritating
Classification	not irritating
Method	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	1981
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Ethanol was applied to six shaved New Zealand white albino rabbits for 4 hours under exposure chamber of 6 cm2. Draize scoring criteria. Mean score for erythema was 1.0 after 1 and 24 hours. Scores for erythema and oedema were 0.0 at all other time points.
Reliability	(2) valid with restrictions
Flag	Critical study for SIDS endpoint
Reference	Monick, JA (1968) in Alcohols. Their Chemistry Properties and Manufacture. Reinhold 1969, LCCCN 68-23906: p. 75.
17.11.2004	(185)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rabbit
Concentration	95%
Exposure	
Exposure time	
Number of animals	4
Vehicle	Water
PDll	
Result	slightly irritating
Classification	not irritating
Method	other
Year	1971
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Classification according to Directive 67/548/eei: is not possible

	from the data presented in this paper. Method was a modified Draize test employing groups of 4 rabbits and 24-hour covered application. The average score was 0.5 out of a possible 8 (scores of 0.62, 0.62 and 0.25 were recorded for 3 repetitions). Test compound was 95% ethanol.
Reliability	(2) valid with restrictions
Reference	Phillips, L. II., Steinberg, M., Maibach, H.J., Akers, WA (1972) A comparison of rabbit and human skin response to certain irritants. Toxicol Appl Pharmacol 21:369-382.
12.11.2004	(186)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rabbit
Result	not irritating
Classification	
Method	other
Year	1979
GLP	No
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	After Fed Reg vol 38 No 187 27-05-1973 1500.41
Reliability	(4) not assignable
Reference	BASF AG Toxicology Department unpublished research (78/810-Sill) 04-09-1979.
12.11.2004	(187)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rabbit
Result	not irritating
Classification	
Method	Draize Test
Year	1978
GLP	No
Test substance	ethanol (64-17-5)
Remark	ethanol 96%
Reliability	(4) not assignable
Reference	BASF AG Toxicology Department unpublished research TNO Report No R5724 (1978).

12.11.2004 (188)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Human
Concentration	Undiluted
Exposure	Occlusive
Exposure time	4 hour(s)
Number of subjects	31
Vehicle	
PDll	
Result	not irritating
Classification	not irritating
Method	other
Year	2004
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Application of 0.2ml ethanol on a 25mm plain Hill Top chamber containing a Webrll pad to the skin of human volunteers for 4 hours. Full details given in York (1996)) and Basketter (1.997), Treatment sites assessed for irritation on a four point scale at 24, 48 and 72hrs after pad removal. Any weakly positive reaction (mild erythema or dryness across most of contact site) considered a positive reaction. Interpretation of results in terms of EU classification done by statistical comparison with a concurrent positive control (20% sodium dodecyl sulphate). One out of 31 subjects produced a positive result. Positive control produced a reaction in 15 out of 31 subjects Ethanol therefore considered non-irritant.
Reliability	(4) not assignable
Reference	Basketter DA. York M, McFadden JP, Robinson MK (2004) Determination of skin irritation potential in the human 4-hour patch test. Contact Dermatitis 51, 1-4.

17.11.2004 (189)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance:	Identity: 1-Butanol, Union Carbide sample procured 12120/48 from Fellowship 155.
Method:	Internal Union Carbide method for skin irritation.
Test type:	Rabbit belly vesicant test (uncovered).
GLP:	No

Year performed:	Not specified.
Species/strain:	Rabbit
Sex:	Not specified.
Number of animals/ sex/dose:	Not specified.
Vehicle:	None
Route of admin. :	Undiluted n-butanol was applied to the belly of rabbits and left uncovered.
Results:	No irritation was observed. Graded 1 on a scale of 1 to 10.
Comments:	No further details available.
Data quality:	Reliability: Key study. Klimisch quality 2.
References:	Union Carbide Corp. Bushy Run Research Center, Proj ect Report No.14-73. Export, P A. 1951.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance:	1-butanol
Test species/strain:	Rabbit
Test method:	Not Stated
GLP:	No
Test results:	405 mg/24-Hr. Moderate skin irritation observed.
Comments:	
Reference:	US DHEW. 1978. Registry of toxic effects of chemicals, Washington DC, US Department of Health, Education and Welfare. As cited in World Health Organization (WHO). 1987. Environmental Health Criteria 65: Butanols - Four Isomers: 1Butanol 2-Butanol tert-Butanol Isobutanol. WHO. Registry of Toxic Effects of Chemical Substances. p.1301, 1985-86.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance:	1-Butanol
Test species/strain:	Rabbit
Test method:	Not Stated
GLP:	No
Test results:	500 mg/24-Hr. Moderate skin irritation observed.
Comments:	
Reference:	US DHEW. 1978. Registry of toxic effects of chemicals, Washington DC, US Department of Health, Education and Welfare. As cited in World Health Organization (WHO). 1987. Environmental Health Criteria 65: Butanols - Four Isomers: 1-Butanol 2-Butanol tert-Butanol Isobutanol. WHO. Registry of Toxic Effects of Chemical Substances. p.1301, 1985-86.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-butanol
Test species/strain: Human
Test method: Occupational observation
GLP: No

Test results: Dermatitis of the fingers and hands has been described after exposure to 1-butanol. Other observations noted included fissured eczema around fingernails and along the sides of fingers.
Comments:
Reference: Tabershaw LR., Fahy J.P. and Skinner J.B. Industrial exposure to butanol. Ind. Hyg. Toxicol. 26:328-331. 1944.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species/strain: Human
Test method: Chamber Test method
GLP:
Test results: 105 patients were tested for 1-butanol induced non immunological contact urticaria. 20 µl of undiluted 1-butanol was applied to the upper back with an occlusive patch for 20 minutes. No redness was observed in any subject. 4 patients were positive for edema.
Comments:
Reference: Lahti A. Nonimmunologic contact urticaria. Acta. DermatoVenereol. Suppl.,60 (91): 1-49.1980.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: rabbit
Concentration: undiluted
Exposure: Occlusive
Exposure Time: 4 hour(s)
No. of Animals: 6
Vehicle: other: undiluted
Result: irritating
EC classificat.: irritating

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1987
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: AVERAGE SCORE Group mean 24+48+72 hour

- Erythema: 2.13 (72 hour score 2.2)
- Edema: 0.6 (72 hour score 0)

(individual scores were not reported) Erythema and oedema were observed at 1 hour post-exposure.

REVERSIBILITY: Oedema had reduced to 0 at 48 and 72 hours. Erythema reached a maximum of 2.2 at 48 hours persisting at this level to 72 hours.

OTHER EFFECTS: None reported

Source: Jacobs & Martens, 1987
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6
- Controls: No

ADMINISTRATION/EXPOSURE 4 hour exposure
- Preparation of test substance: Undiluted
- Area of exposure: 6 cm2
- Occlusion: Under and exposure chamber
- Vehicle: Undiluted
- Postexposure period: 72 hours
- Removal of test substance: Not reported

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24 , 48 and 72 hours after end of application.

Conclusion: Based on a group mean 24+48+72 hour erythema score of >2

(2.13) 1-hexanol would be classified as irritant according to EU criteria. Although individual scores are not reported 6 animals were used and it is considered that 1-hexanol will be classified as a mild irritant according to GHS criteria.

Cited in Iucldi 2000

Reliability: (2) valid with restrictions
Guideline study without detailed documentation.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau

hexan-1-ol Cas# 111-27-3

Jacobs, G.A. & Martens, M.A., 1987 Skin and eye irritation tests on hexanol. J. Am .Coll. Toxicol. Acute Toxicity Data 11(6):722.

15-JUL-2005 (29) (30)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: rabbit
Concentration: undiluted
Exposure: Occlusive
Exposure Time: 24 hour(s)
No. of Animals: 6
Vehicle: other: undiluted
PDII: 3.58
Result: moderately irritating
EC classificat.: irritating

Method: Draize Test
Year: 1977
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: AVERAGE SCORE 24+48+72 hour
- Erythema: Intact skin 2.03, abraded skin 2.30 (72 hour score intact 2.2, abraded 2.6) Individual scores 3/6 >= 2.3 intact, 4/6 for abraded.
- Oedema: Intact skin 1.23, abraded skin 1.93 (72 hour score intact 0.7, abraded 1.3)

REVERSIBILITY: Over the observation period (72 hours) erythem increased in 4 rabbits while oedema reduced in all rabbits.

OTHER EFFECTS: At 24 and 48 hours the skin at the treatment site in 4 rabbits showed moderate to marked diffuse blanching, with a more intense reaction involving or immediately surrounding the abraded skin.

Source: Scientific Associates, Inc. 1977c
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported

- Number of animals: 6
- Controls: No

ADMINISTRATION/EXPOSURE 24 hour application to intact and abraded skin.
- Preparation of test substance: As a suspension.
- Area of exposure: 1 inch square
- Occlusion: Occlusive
- Vehicle: undiluted
- Postexposure period: 72 hours
- Removal of test substance: Washed off the treated skin (no further details).

EXAMINATIONS
- Scoring system: Draize et al, 1944
- Examination time points: 24, 48 and 72 hours after application.

Test substance: Tradename Alfol 6

Conclusion: Based on the erythema scores reported Alfol 6 is a skin irritant according to EU criteria. 24+48+72 hour mean score of 2.03 for intact and 2.3 for abraded skin. In the absence of information later than 72 hours post exposure Alfol is also considered an irritant according to GHS criteria.

Cited in Iuclid 2000.

Reliability: (2) valid with restrictions
Standard Draize test, reasonably documented, however the test was terminated at 72 hours when there was still marked irritation.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3

Scientific Associates, Inc. 1977c. Acute oral toxicity (LD50) in rats; Acute dermal toxicity (LD50) in rabbits, Dermal irritation test in rabbits; Eye irritation test in rabbits; Inhalation toxicity tests in rats: ALFOL 6. S.A. Number 233619.

11-NOV-2004 (29) (62)

<u>1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)</u>

Species: rabbit
Concentration: 6 %
Exposure: Occlusive
Exposure Time: 24 hour(s)
Vehicle: other: mineral oil
PDII: 1.16

Result: slightly irritating
EC classificat.: not irritating

Method: other: presume Draize
Year: 1970
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: The result of this study was reported as a primary irritation index (PII) which was 1.16. No other study details were available. A PII score of 1.16 would not trigger classification as irritant using either the EU classification system or GHS. Hexanol tested in mineral oil can therefore be considered as at most mildly irritating (GHS category 3) and non-irritant according to EU criteria.
Source: Procter and Gamble 1970.

Hayes Consultancy Service Bromley, Kent
Test condition: TEST ANIMALS: Rabbit
- Strain/sex/source/age/weight: not reported
- Number of animals: Not reported
- Controls: None

ADMINISTRATION/EXPOSURE
From the age of the study and the fact that it was carried out in the USA this is likely to be a Draize test with 24 hour exposure.
- Occlusion: Reported as a patch test
- Vehicle: mineral oil
- Concentration in vehicle: 6%
- Total volume applied: Not reported
- Postexposure period: Not reported

EXAMINATIONS
- Scoring system: Not reported presume Draize, results reported as PII.
- Examination time points: Not reported

Conclusion: From the limited data available 1-hexanol (6% in mineral oil) is not a skin irritant according to EC or GHS criteria.
Reliability: (4) not assignable
Documentation insufficient for assessment.
Flag: Critical study for SIDS endpoint
Reference: Procter and Gamble. 1970. Rabbit skin irritation patch test. Study No. V2674-185.
13-OCT-2004 (50)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: rabbit
Concentration: 100 %
Exposure: Occlusive
Exposure Time: 6 day(s)
No. of Animals: 5
Vehicle: other: undiluted
Result: highly irritating

Method: other: repeated skin application
Year: 1963
GLP: no
Test substance: other TS: 1-hexanol, 2-octanol, 1-heptanol, n-nonanol, n-decanol

Result: The development of the irritative response was similar for all of the alcohols tested. There was a slight reddening of the skin on the initial days following application which developed by days 5-6 to marked redness and inflammation of the skin with the formation of deep cracks. The skin healed witin 10-12 days with the formation of numerous scabs, followed by exfoliation and marked skin pigmentation. Irritation was most marked with n-hexanol and 2-octanol and least marked with n-decanol.
Source: Zaeva, 1963 reported in BIBRA, 1995. Clayton and Clayton, 1994.

Hayes Consultancy Service Bromley, Kent
Test condition: Groups of 5 rabbits received a daily topical application of 2 ml undiluted alcohol to the shorn skin for 6 days, no further experimental details were available. No individual scores were reported. Four primary alcohols were tested n-hexanol, n-heptanol, n-nonanol and n-decanol. Also tested was the secondary alcohol 2-octanol.
Conclusion: Repeated application of C6, 7, 8, 9 and 10 alcohols to rabbit skin for 6 consecutive days resulted in marked irritation with eschar. The most marked irritation was seen with n-hexanol and 2-octanol, the least irritation was observed with n-decanol. Also reported by BIBRA, 1995. Clayton and Clayton, 1994.
Reliability: (2) valid with restrictions
Non-standard test with limited documentation. Useful for supporting information.
Reference: Clayton, G.D. and Clayton, F.E. (eds.). Chapter 55 Alcohols 1994. Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc.

Zaeva, G.N. and Fedorova, V.I 1963 The toxicology of higher saturated monoatomic alcohols (n-hexyl, n-heptyl, n-octyl, n-nonyl and n-decyl). Toksikol. Novykh. Prom. Khim. Vesch. 5:51-55.
15-JUL-2005 (17) (85)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: other: rabbit, guineapig, hairless mouse, human volunteers
Concentration: 50 %
Exposure: Occlusive
Exposure Time: 24 hour(s)
No. of Animals: 4
Vehicle: other: vaseline

Method: other
Year: 1977
GLP: no
Test substance: other TS: even C6-22 alcohols

Result: The most marked skin reactions were observed with rabbits, the degree of irritancy was related to carbon chain length. Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12) to a maximum class 5 at C14, then reducing to class 3 at C16 & 18. The human scores generally were less than those of the rabbits and reached a peak of class 3 with the C10 alcohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with hairless mouse skin. The response in guinea pigs followed no obvious pattern and all scores were classed as <=3.

In some cases alcohols have been given descriptive ratings for rabbits and man in Iuclid datasets. These ratings together with the actual gradings from this reference are reported below.

1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol) reaction class 3 for rabbits and 2 for man (Kaestner 1977).
1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).

Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

Source: Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

Test condition: In this comparative study C6-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. All applications were made at a concentration of 50% in vaseline. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the

group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

Conclusion: This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible. N-hexanol applied as 50% in vaseline produced practically no skin irritation in rabbits, hairless mice and human volunteers and marginal irritation in guineapigs.

Cited in Iuclid 2000.

Reliability: (2) valid with restrictions
Comparative study meeting generally accepted scientific principles.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau
hexan-1-ol Cas# 111-27-3

Kaestner, W. 1977. Zur Speziesabhangigkeit der

Hautvertraglichkeit von Kosmetikgrundstoffen. J. Soc. Cos. Chem. 28: 741-754.
11-NOV-2004 (29) (31)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: rabbit
Result: moderately irritating
EC classificat.: irritating

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1986
GLP: no data
Test substance: other TS: Nacol 6 RD 1-hexanol (111-27-3)

Reliability: (4) not assignable
Secondary reference to study carried out to OECD 404 for Condea Chimie GmbH, original unavailable.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3
13-OCT-2004 (29)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Remark: Cited in Iuclid 2000 as Henkel report TBD 910457 which is unavailable. Irritation study in rabbits, no further details reported. Described as moderately irritating.
Test substance: 1-hexanol
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3
13-OCT-2004 (29)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Remark: Summary data cited by RTECS obtained from Union Carbide Data Sheet, 1967. 410 mg of n-hexanol was applied to rabbit skin in an open irritation test. The degree of irritation was described as mild. No further details available, original unobtainable.
Reliability: (4) not assignable
Secondary reference
Reference: RTECS, 2004.
13-OCT-2004 (55)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Species: rabbit
Concentration: undiluted
Exposure: Semiocclusive
Exposure Time: 4 hour(s)
No. of Animals: 3
Vehicle: other: none
Result: slightly irritating
EC classificat.: not irritating

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1992
GLP: yes
Test substance: > 90% 1-octanol (111-87-5)

Result: AVERAGE SCORE
- Erythema: Individual mean 24+48+72 hour scores 1.0, 2.0 and 1.3. Group mean 24+48+72 hour score 1.43.
- Edema: All scores 0.

REVERSIBILITY: By day 7 all erythema and oedema scores were 0.

OTHER EFFECTS: The test site was sticky to touch at 1 hour post-dosing. A loss of elasticity at the test site was reported at 48 and 72 hours. From day 7 until the end of the observation period (day 16) exfoliation was observed in all test animals. Control sites showed no skin irritation all scores 0.

Source: Johnson 1996a; OECD 1987b.

Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Female
- Source: Froxfield SPF Rabbits, Hampshire, UK
- Age: ca 3 months
- Weight at study initiation: 2.22 - 2.64 kg
- Number of animals: 3

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 3X2 cm
- Occlusion: semi-occlusive
- Vehicle: None
- Total volume applied: 0.5 ml

- Exposure period: 4 hours
- Postexposure period: 16 day
- Controls: The other flank of the animal was used as a control site.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours post application then at 7, 10, 13 and 16 days.

Conclusion: The C8 alcohol Kalcohl 0898 is not a skin irritant according to either EU criteria following a 4 hour semi-occlusive exposure. Kalcohl 0898 can be considered as a mild irritant under GHS criteria.

Reliability: (1) valid without restriction
Guideline study.

Flag: Critical study for SIDS endpoint

Reference: Johnson, I.R. 1996a. Kalcohl 0898: Acute dermal irritation test in the rabbit. Amended final report. Report No. 96/KAS214/0952.

11-MAY-2006 (67)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Species: other: rabbit, guineapig, hairless mouse, human volunteers
Concentration: 50 %
Exposure: Occlusive
Exposure Time: 24 hour(s)
No. of Animals: 4
Vehicle: other: vaseline

Method: other
Year: 1977
GLP: no
Test substance: other TS: even C6-22 alcohols

Result: Result : The most marked skin reactions were observed with rabbits, the degree of irritancy was related to carbon chain length. Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12)to a maximum class 5 at C14, then reducing to class 3 at C16 & 18. In most cases the human scores were less those of the rabbits and reached a peak of class 3 with the C10 aclohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with hairless mouse skin. The response in guineapigs followed no obvious pattern and all scores were classed as

<=3.

The results for C8, C12, C14, C16 and C18 alcohols have been given descriptive ratings for rabbits and man in some Iuclid datasets on aliphatic alcohols and these ratings together with the actual gradings from this reference are reported below.

1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol); reaction class 3 for rabbits and 2 for man (Kaestner 1977).
1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).
Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)

Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

Source: Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

Test condition: In this comparative study C4-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. The test substance was applied at 50% in vaseline. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

Conclusion: This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin

reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible.

Reliability: (2) valid with restrictions
Comparative study meeting generally accepted scientific principles.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Octan-1-ol Cas# 111-87-5.

Kaestner, W. 1977. Zur Speziesabhangigkeit der Hautvertraglichkeit von Kosmetikgrundstoffen. J. Soc. Cos. Chem. 28:741-754.

18-OCT-2004 (62) (70)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Remark: This report of skin irritation with n-octanol is reported in several secondary references. These sources are erroneous, the original report in Patty 1963 of an unpublished reference by Fassett is clearly an assessment for 2-octanol. This data does not appear in Patty 2001.

Test substance: 2-octanol

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Octan-1-ol Cas# 111-87-5.

Opdyke, D.L.J. 1973 Monographs on fragrance raw materials. Fd. Cos. Tox. 11:95-115.

RTECS, 2004.

17-OCT-2004 (62) (88) (93)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Remark: Undiluted C8-alcohol applied undiluted to intact or abraded rabbit skin was reported to produce mild skin irritation. No further experimental details were available from this secondary reference to unpublished data provided by Levenstein, 1972.

Source: Opdyke, 1973a

Test substance: Reported as a C8 alcohol (1-octanol)

Reliability: (4) not assignable
Secondary reference.

Reference: Opdyke, D.L.J. 1973a Fragrance raw materials monographs. Supplement to earlier monographs on fragrance raw materials.

Fd. Cos. Tox. 11: 1011-1081.

RTECS, 2004
11-NOV-2004 (89) (93)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Remark: 2% 1-octanol in petrolatum did not cuse irritation to human skin following a 48 hour closed application. 25 volunteers were tested. No further details available from this secondary report of unpublished data provided by Kligman, 1972.
Test substance: 1-octanol
Reliability: (4) not assignable
Secondary reference.
Reference: Opdyke, D.L.J. 1973a Fragrance raw materials monographs. Supplement to earlier monographs on fragrance raw materials. Fd. Cos. Tox. 11:1011-1081.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.
11-NOV-2004 (89) (90)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Species: rabbit
Exposure: Semiocclusive
Exposure Time: 4 hour(s)
No. of Animals: 3
Vehicle: other: undiluted
Result: irritating
EC classificat.: irritating

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1996
GLP: yes
Test substance: > 90% 1-decanol (112-30-1)

Result: AVERAGE SCORE
- Erythema: Individual 24+48+72 hour scores 1.7, 2.0, 2.0 (Group mean score 1.9)
- Oedema: All scores 0

REVERSIBILITY: At 7 days one animal only exhibited erythema. By 10 days all scores were 0 and the skin appeared normal.

OTHER EFFECTS: Loss of elasticity was reported at 48 and 72

hours after removal of the dressings. Control sites showed no evidence of skin irritation.

Source: Johnson 1996b
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbits
- Strain: out bred New Zealand white
- Sex: Female
- Source: Froxfield SPF Rabbits, Hampshire, UK
- Age: ca 3 months
- Weight at study initiation: 2.32-2.51 kg
- Number of animals: 3
- Controls: Untreated patches on same animals.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 3X2 cm
- Occlusion: semioccluded
- Vehicle: none
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 10 days
- Removal of test substance: warm water & paper tissues after 4 hours

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours after dressing removal and at 7 and 10 days.

Test substance: Tradename Kalcohl 1095

Conclusion: In this 4 hour semi-occlusive study Kalcohl 1095 (C12) would be considered a skin irritant under EU criteria with a mean 24+48+72 hour erythema score for 2 animals of >=2. Under GHS criteria this alcohol would be considered a mild irritant (category 3).

Reliability: (1) valid without restriction
Comparative study meeting generally accepted scientific principles.

Flag: Critical study for SIDS endpoint

Reference: Johnson, I.R. 1996b. Kalcohl 1095: Acute dermal irritation test in the rabbit. Final report. Report No. 96/KAS220/0677.

05-AUG-2005 (56)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Species: rabbit

Exposure: Semiocclusive
Exposure Time: 4 hour(s)
No. of Animals: 4
Vehicle: other: undiluted
PDII: 3.33
Result: moderately irritating

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1996
GLP: yes
Test substance: > 90% 1-decanol (112-30-1)

Method: The in vivo data were generated in studies carried out since 1981 according to OECD Test guideline 404. The skin irritation data were collected from various sources to provide a reference data bank for validation of alternative skin testing methods. The data were obtained from tests normally using at least three rabbits evaluated at the same time involving applications of 0.5 g or 0.5 mL to the flank under semi-occlusive patches for 4 hours and in which observations were made at least 24, 48, and 72 hours after removal of the patch.

In the case of 1-decanol 4 rabbits were tested with undiluted 1-decanol of 98% purity. Observations were continued to 7 days.

Result: AVERAGE SCORE 24+48+72 hour
- Erythema: Individual 2.3; 2.3; 2.2; 1.8 Mean 2.15
- Oedema: Individual 2.0; 0.8; 1.0; 0.8 Mean 1.15

PII based on 24, 48 and 72 hour scores 3.33.

REVERSIBILITY: 7 days scores
- Erythema: Individual 1; 1; 2; 2 Mean 1.5
- Oedema: Individual 0; 0; 0.5; 0.5 Mean 0.25

OTHER EFFECTS: Desquamation was observed at all test sites at 7 days, this was described as marked in one animal.

Source: Bagley 1996.
Hayes Consultancy Service Bromley, Kent

Conclusion: Based on individual mean 24+48+72 hour scores of 2.3 for erythema in 2 of the 4 test animals plus persistence of the response to 7 days with desquamation in all animals it is considered that 1-decanol is irritating (Category 2) to the skin according to the GHS system and irritant according to EU criteria based on a group mean 24+48+72 hour score of 2.15 for

erythema.
Reliability: (1) valid without restriction
Compilation of data conducted to OECD guidelines, reported in summary by Bagley, 1996 however full results available in ECETOC Technical Report No. 66, 1995.
Flag: Critical study for SIDS endpoint
Reference: Bagley, D.M., Gardner, J.R., Holland, G., Lewis, R.W., Regnier, J-F., Stringer, D.A., and Walker, A.P. 1996. Skin irritation: Reference chemicals data bank. Toxicity in Vitro 10:1-6.

ECETOC, 1995 Skin irritation and corrosion: Reference chemicals data bank. ECETOC Technical Report No. 66.
05-AUG-2005 (9) (26)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Species: rabbit
Concentration: 100 %
Exposure: Occlusive
Exposure Time: 8 hour(s)
No. of Animals: 5
Result: slightly irritating
EC classificat.: not irritating

Method: other
Year: 1979
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Result: No individual scores are given. The test material is reported as producing slight irritation which is reversible over the 14 day observation period. A score of 2,2 is reported but it is not clear exactly what this refers to.
Source: Potokar, 1979
Hayes Consultancy Service Bromley, Kent
Test condition: TEST ANIMALS:
- Strain: Albino rabbits
- Sex: Male
- Age: Adult
- Number of animals: 5

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: Not reported
- Occlusion: Yes

- Vehicle: None
- Exposure period: 8 hours
- Postexposure period: 14 days
- Removal of test substance: Not reported.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: immediately after removal of patch then at 24 hours, observed until 14 days.

Test substance: Tradename Lorol 10.
Conclusion: Based on the limited data available it is considered that Lorol 10 is slightly irritating to the skin but unlikely to be a skin irritant under GHS or EU criteria.
Reliability: (4) not assignable
Documentation limited and insufficient for assessment but study appears a reasonably conducted standard Draize test.
Flag: Critical study for SIDS endpoint
Reference: Potokar, 1979. Lorol 810 und Lorol C 10, toxikologische Untersuchungen. No. 281. 27 November 1979.
05-AUG-2005 (71)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Species: other: rabbit, guineapig, hairless mouse, human volunteers
Concentration: 50 %
Exposure: Occlusive
Exposure Time: 24 hour(s)
No. of Animals: 4
Vehicle: other: vaseline

Method: other
Year: 1977
GLP: no
Test substance: other TS: even C6-22 alcohols

Result: The most marked skin reactions were observed with rabbits, the degree of irritancy was related to carbon chain length. Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12)to a maximum class 5 at C14, then reducing to class 3 at C16 & 18. In all cases the human scores were less those of the rabbits and reached a peak of class 3 with the C10 aclohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with hairless mouse skin. The response in guineapigs followed no obvious pattern and all scores were classed as <=3.

The results for C8, C12, C14, C16 and C18 alcohols have been given descriptive ratings for rabbits and man in various Iuclid datasets on aliphatic alcohols and these ratings (where available) together with the actual gradings from this reference are reported below.
1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol); reaction class 3 for rabbits and 2 for man (Kaestner 1977).
1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).
Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

Source: Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

Test condition: In this comparative study C4-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

Conclusion: This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible.

Reliability: (2) valid with restrictions
Comparative study well documented, meets generally accepted scientific principles, acceptable for assessment but not for classification.
Reference: Iuclid 2000 ECB Decanol.

Kaestner, W. 1977. Zur Speziesabhangigkeit der Hautvertraglichkeit von Kosmetikgrundstoffen. J. Soc. Cos. Chem. 28: 741-754
05-AUG-2005 (53) (58)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Species: rabbit
Concentration: 100 %
Exposure: Occlusive
Exposure Time: 6 day(s)
No. of Animals: 5
Vehicle: other: undiluted
Result: highly irritating

Method: other: repeated skin application
Year: 1963
GLP: no
Test substance: other TS: 1-hexanol, 2-octanol, 1-heptanol, n-nonanol, n-decanol

Result: The development of the irritative response was similar for all of the alcohols tested. There was a slight reddening of the skin on the initial days following application which developed by days 5-6 to marked redness and inflammation of the skin with the formation of deep cracks. The skin healed witin 10-12 days with the formation of numerous scabs, followed by exfoliation and marked skin pigmentation. Irritation was most marked with n-hexanol and 2-octanol and least marked with n-decanol.
Source: Zaeva, 1963 reported in BIBRA, 1995. Clayton and Clayton, 1994.
Hayes Consultancy Service Bromley, Kent
Test condition: Groups of 5 rabbits received a daily topical application of 2 ml undiluted alcohol to the shorn skin for 6 days, no further experimental detaols were available. No individual scores were reported. Four primary alcohols were tested n-hexanol, n-heptanol, n-nonanol and n-decanol. Also tested was the secondary alcohol 2-octanol.
Conclusion: Repeated application of C6, 7, 8, 9 and 10 alcohols to rabbit

skin for 6 consecutive days resulted in marked irritation with eschar. The most marked irritation was seen with n-hexanol and 2-octanol, the least irritation was observed with n-decanol.

Reliability: (2) valid with restrictions
Non-standard test with limited documentation.

Reference: BIBRA. 1995. Toxicity Profile: 2-Octanol. BIBRA International.

Clayton, G.D. and Clayton, F.E. (eds.). Chapter 55 Alcohols 1994. Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc.

Zaeva, G.N. and Fedorova, V.I. 1963 The toxicology of higher saturated monoatomic alcohols (n-hexyl, n-heptyl, n-octyl, n-nonyl and n-decyl). Toksikol. Novykh. Prom. Khim. Vesch. 5:51-55.

08-OCT-2004 (16) (21) (106)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Remark: Report of a Czech publication, 1986. Very limited data, a 24 hour application of 20 mg test substance to the skin caused moderate irritation. No further details available.

Test substance: Decyl alcohol isomeric content not reported

Reliability: (4) not assignable
Secondary reference, original unavailable.

Reference: RTECS on line 2004 Decyl Alcohol.

05-AUG-2005 (74)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Species: human
Concentration: undiluted
Exposure: Occlusive
Exposure Time: 4 hour(s)
No. of Animals: 30
Result: not irritating

Method: other: human 4-hr patch test
Year: 1998
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Result: Decanol produced a minimal response on human skin equivalent to that produced by water.

Source: Robinson et al, 1998

Test condition: O.2 ml undiluted decanol was applied to the skin of human volunteers for up to 4 hours using a 25mm Hill Top chamber held in place with adhesive tape. The test site was scored on a 4 point scale. Once a positive response was observed in a given subject there was no further exposure to the material. A the end of the exposure excess material at the test site was removed using a damp towel. Sodium dodecyl sulphate was used as a positive control.

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Reference: Robinson, M.K. Applicatin of a 4-hr human patch test method for comparative and investigative assessment of skin irritation. Contact Dermatitis 38:194-202.

05-AUG-2005 (73)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Species	:	other: New Zealand White rabbit
Concentration	:	
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	3
PDII	:	3.5
Result	:	moderately irritating
EC classification	:	irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1996
GLP	:	yes
Test substance	:	dodecanol (112-53-8)
Test substance	:	Tradename Kalcol 2098
Test condition	:	TEST ANIMALS: Rabbits - Strain: New Zealand White - Sex: Male - Source: David Percival Ltd, Cheshire, UK - Age: 12-16 weeks - Weight at study initiation: 2.44-2.67 kg - Number of animals: 3 - Controls: Not reported ADMINISTRATION/EXPOSURE - Preparation of test substance: The test substance was a white crystalline solid which was warmed to 40C before application. - Area of exposure: 2.5x2.5 cm

- Occlusion: semi-occlusive
- Vehicle: None applied undiluted
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 14 days
- Removal of test substance: Swabbing with cotton wool soaked in 74% methylated spirits.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours after patch removal and at 7 and 14 days.

Result : AVERAGE SCORE
- Erythema: Individual 24+48+72 hour scores were 2 for each animal. Group mean 24+48+72 hour score 2. The reaction extended beyond the treatment site.
- Oedema: Individual 24+48+72 hour scores were 1.7 for each animal. Group mean 24+48+72 hour score 1.7.

The PII was 3.5 (moderately irritating)

REVERSIBILITY: Crust formation in all test animals at 7 days prevented the accurate evaluation of erythema. There was no oedema. By 14 days all erythema scores were 0.

OTHER EFFECTS: Slight desquamation was noted in all animals at 14 days.

Conclusion : Following a 4 hour semi-occlusive application to rabbit skin Kalcohl 2098 was a skin irritant accordng to EU criteria (group mean 24+48+72 hour score 2). Based on erythema and oedema scores Kalcohl 2098 is a mild irritant (category 3) under GHS criteria.

Reliability : (1) valid without restriction
Guideline study

Source : Sanders 1996a
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference SIDS Dossier on 1-Dodecanol. 1993a. Environmental Protection Agency, Denmark. 6 June 1993.

11.08.2005 (19)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)</u>

Species : rabbit

Concentration	:	10 % active substance
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	3
PDII	:	1.3
Result	:	not irritating
EC classification	:	not irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1997
GLP	:	yes
Test substance	:	dodecanol (112-53-8)
Test substance	:	Tradename Kalcol 2098
Test condition	:	TEST ANIMALS: Rabbits - Strain: New Zealand White - Sex: Male - Source: David Percival Ltd, Cheshire, UK - Age: 12-16 weeks - Weight at study initiation: 2.71-2.90 kg - Number of animals: 3 - Controls: Not reported ADMINISTRATION/EXPOSURE - Preparation of test substance: The test substance was a white crystalline solid which was prepared as a 10% solution in PEG 400 - Area of exposure: 2.5x2.5 cm - Occlusion: semi-occlusive - Vehicle: polyethylene glycol 400. - Total volume applied: 0.5 ml - Exposure period: 4 hours - Postexposure period: 14 days - Removal of test substance: Swabbing with cotton wool soaked in distilled water. EXAMINATIONS - Scoring system: Draize - Examination time points: 1, 24, 48 and 72 hours after patch removal and at 7 and 14 days.
Result	:	AVERAGE SCORE - Erythema: Individual mean 24+48+73 hour scores 0, 1.3, 1.7. Group mean 24+48+72 hour score 1. - Edema: Individual mean 24+48+73 hour scores 0, 0.3, 0.7. Group mean 24+48+72 hour score 0.3.

REVERSIBILITY: All scores were 0 at 7 days and all test sites appeared normal at 14 days.

OTHER EFFECTS: The erythema extended beyond the test site in 2 rabbits at 24 and 48 hours. Desquamation (moderate) was observed in one of these rabbits at 7 days.

Conclusion : Following a 4 hour semi-occlusive exposure to rabbit skin a 10% solution of Kalcol 2098 in PEG 400 would not be considered irritant by either EU or GHS criteria. The group mean 24+48+72 hour scores for erythema and oedema were 1 and 0.3 respectively. The individual 24+48+72 hour scores did not exceed 1.5 in more than one rabbit.

Reliability : (1) valid without restriction
Guideline study

Source : Hempstock, 1997a

Flag : Critical study for SIDS endpoint

Reference Henkel KGaA. 1994d. Lorol C12-99: Algen-Zellvermehrungshemmtest. Biological Research and Product safety/Ecology: Unpublished results; Report No. R 9400362.

11.08.2005 (10)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Species : human

Concentration : undiluted

Exposure : Semiocclusive

Exposure time : 4 hour(s)

Number of animals : 20

PDII :

Result : not irritating

EC classification : not irritating

Method : other: patch test baed on OECD 404

Year : 1996

GLP : yes

Test substance : dodecanol (112-53-8)

Test substance : Tradename Lorol C12-98

Test condition : The effect on human skin was investigated:
15 drops/plaster of undiluted test substance were added to a semi-occlusive plaster (diameter: 1.5 cm) and applied for 4 hours to the backs of healthy volunteers. Readings of erythema, edema, scaling and fissures were taken 1, 24, 48 and 72 hours after application. 20 male and female volunteers were tested. Age was 22 - 53 years with

an average of 34.9 years.

Study was performed under Good Clinical Practice (GCP).

Result : No irritation was observed following application to the human skin of undiluted test substance for 4 hours (patch test).

Conclusion : Undiluted Lorol C12-98 did not produce any skin irritation in human vounteers following a 4 hour semi-occlusive exposure in a test based on OECD 404.

Reliability : (1) valid without restriction
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.

Reference Henkel KGaA. 1999q. Dodecanol: Acute toxicity Daphnia. Unpublished data, Test substance registration no. 910724.

25.10.2005 (11)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Species : human
Concentration : undiluted
Exposure : Open
Exposure time : 1 hour(s)
Number of animals : 20
PDII :
Result : not irritating
EC classification : not irritating
Method : other: Burckhardt test, open epicutaneous
Year : 1996
GLP : yes
Test substance : dodecanol (112-53-8)

Test substance : Tradename Lorol C12-98

Test condition : The effect on human skin was investigated:
15 drops/plaster of undiluted test substance were added to a semi-occlusive plaster (diameter: 1.5 cm) and applied for 4 hours to the backs of healthy volunteers. Readings of erythema, edema, scaling and fissures were taken 1, 24, 48 and 72 hours after application. 20 male and female volunteers were tested. Age was 22 - 53 years with an average of 34.9 years.

Study was performed under Good Clinical Practice (GCP).

Result : No irritation was observed following application to the human skin of

undiluted test substance for 4 hours (patch test).

Conclusion : Lorol C12-98 was not irritating to human skin following repeated application to non-occluded skin over a period of 1 hour.

Reliability : (1) valid without restriction
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.

Reference Linden, E., Bengtsson, B.E., Svanberg, O., and Sundstrom, G. 1979. The acute toxicity of 78 chemicals and pesticide formulations against two brackish water organisms. The bleak (Alburnus alburnus) and the harpaticoid Nitocra spinipes. Chemosphere 11-12: 843-851.

25.10.2005 (14)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Species: rabbit
Concentration: 50 %
Exposure: Occlusive
Exposure Time: 24 hour(s)
No. of Animals: 6
Vehicle: other: 1% gum tragacanth
PDII: 4.3
Result: irritating
EC classificat.: irritating

Method: other: contract laboratory protocol
Year: 1977
GLP: no data
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: AVERAGE SCORE 24+48+72 hours
- Erythema: Intact skin 2.43, abraded skin 2.53 (72 hours score intact 2.4, abraded 2.8) Individual scores 5/6 greater than 2.3.
- Oedema: intact skin 1.83, abraded skin 3.26 (72 hours score intact 1.3, abraded 1.5)

REVERSIBILITY: Erythema increased or persisted until 72 hours after application while oedema decreased or persisted.

OTHER EFFECTS: None reported.

Source: Scientific Associates, 1977b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London

Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6
- Controls: No

ADMINISTRATION/EXPOSURE 24 hour application to intact and abraded skin.
- Preparation of test substance: As a suspension.
- Area of exposure: 1 inch square
- Occlusion: Occlusive
- Vehicle: 1% gum tragacanth
- Concentration in vehicle: 50%
- Total volume applied: 1 ml (500 mg Alfol 14)
- Postexposure period: 72 hours
- Removal of test substance: Washed off the treated skin (no further details).

EXAMINATIONS
- Scoring system: Draize et al, 1944
- Examination time points: 24, 48 and 72 hours after application.

Conclusion: Based on the erythema and oedema scores reported Alfol 14 would be considered a skin irritant according to EU criteria and a class 2 irritant according to GHS criteria. Individual 24+48+72 hour erythema scores were >2.3 in 5/6 animals while the group mean 24+48+72 hour score was also in excess of 2.3 (2.46).

Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions. Well documented and conducted study.

Flag: Critical study for SIDS endpoint

Reference: Scientific Associates, Inc. 1977b. Acute oral toxcity (LD50) in rats, acute dermal toxicity (LD50) in rabbits, dermal irritation test in rabbits, eye irritation test in rabbits, and inhalation toxicity test in rats. ALFOL 14 alcohol.

16-JUL-2005 (64)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)</u>

Species: human

Concentration: undiluted
Exposure: Semiocclusive
Exposure Time: 4 hour(s)
No. of Animals: 20
Result: not irritating
EC classificat.: not irritating

Method: other: patch test based on OECD 404
Year: 1996
GLP: yes
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: No irritation was observed following application to the human skin of undiluted test substance for 4 hours (patch test).
Source: Hayes Consultancy Service Bromley, Kent
Test condition: The effect on human skin was investigated: 15 drops/plaster of undiluted test substance were added to a semi-occlusive plaster (diameter: 1.5 cm) and applied for 4 hours to the backs of healthy volunteers. Readings of erythema, edema, scaling and fissures were taken 1, 24, 48 and 72 hours after application. 20 male and female volunteers were tested. Age was 22 - 53 years with an average of 34.9 years. Study was performed under Good Clinical Practice (GCP).
Test substance: Tradename Lorol 14
Conclusion: Lorol C12-98 is not irritating to human skin following a 4 hour semi-occlusive exposure.
Reliability: (1) valid without restriction
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.
Flag: Critical study for SIDS endpoint
Reference: Henkel KGaA, 1996 HD-Ocenol 90/95 V, Lorol C12-98, Lorol-C14-98, Lorol Spezial. 4h Patch Test (in Anlehnung an OECD Guideline Nr. 404). Henkel KGaA 1996, Report No. R 9601427.
25-OCT-2005 (25)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)</u>

Species: human
Concentration: undiluted
Exposure: Open
Exposure Time: 1 hour(s)
Result: not irritating
EC classificat.: not irritating

Method: other: open epicutaneous test according to Burckhardt

Year: 1996
GLP: yes
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: Slight redness was observed after the 1 hour application period which disappeared within 15 minutes.
Source: Hayes Consultancy Service Bromley, Kent
Test condition: The effect on human skin was investigated:
Undiluted test substance was applied to the forearm with a glass rod for a total application period of 60 minutes. Every 30 seconds, the test substance was gently swabbed with tissue and new test substance applied. Objective findings (erythema, edema) and subjective sensations (e.g. itching, cauterization etc.) were recorded after 15, 30, 45 and 60 minutes.
20 male and female volunteers of average age 35.3 years were tested.
Study was performed under Good Clinical Practice (GCP).
Test substance: Tradename Lorol 14
Conclusion: Lorol C12-98 was essentially non-irritating to human skin following repeated application to non-occluded skin over a period of 1 hour.
Reliability: (1) valid without restriction
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.
Reference: Henkel KGaA 1996a Offener Epikutan-Test nach Burckhardt. HD-Ocenol 90/95 V, Lorol C12-98, Lorol-C14-98, Lorol Spezial. Henkel KGaA 1996, Report No. R 9601185.
25-OCT-2005 (24)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Species: rabbit
Concentration: 100 %
Exposure: Occlusive
Exposure Time: 24 hour(s)
Result: not irritating
EC classificat.: not irritating

Method: Draize Test
Year: 1974
GLP: no
Test substance: > 95% 1-Tetradecanol (112-72-1)

Remark: This monograph gives a brief report of a skin irritation study carried out with undiluted 1-tetradecanol using the Draize method with 24 hour occluded application to intact and abraded

rabbits skin. The unpublished data was submitted by Levenstein 1974 and is also reported in Iuclid 2000 adn Patty, 2001.

Result: The undiluted C14 alcohol 1-tetradecanol was reported to be non-irritating to the skin following a 24 hour occluded exposure to intact and abraded rabbits skin. No further experimental details or irritation scores are available.

Source: Opdyke, 1975
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Tetradecanol Cas# 112-72-1.

Opdyke, D.L.J. 1975 Fragrance raw material monographs - Alcohol C14 Myristic. 13(Suppl.) 699-700.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

25-OCT-2005 (44) (53) (54)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Species: human
Concentration: 12 %
Exposure: Occlusive
Exposure Time: 48 hour(s)
Vehicle: petrolatum
Result: not irritating

Method: other
Year: 1974
GLP: no
Test substance: > 95% 1-Tetradecanol (112-72-1)

Remark: This monograph gives a brief report of a skin irritation study carried out with undiluted 1-tetradecanol on human skin. 1-tetradecanol was tested against 2 panels of human subjects using a 48 hour closed patch test. This is a report of unpublised data provided by Kligman, 1974.

Result: 1-tetradecanol did not cause irritation to human skin following a 48 hour closed-patch exposure.

Source: Opdyke, 1975
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London

Hayes Consultancy Service Bromley, Kent
Reliability: (4) not assignable
Secondary reference.
Reference: Opdyke, D.L.J. 1975 Fragrance raw material monographs - Alcohol C14 Myristic. 13(Suppl.) 699-700
25-OCT-2005 (53)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Species: other: rabbit, guineapig, hairless mouse, human volunteers
Concentration: 50 %
Exposure: Occlusive
Exposure Time: 24 hour(s)
No. of Animals: 4

Method: other
Year: 1977
GLP: no
Test substance: other TS: even C6-22 alcohols

Result: The most marked skin reactions were observed with rabbits, the degree of irritancy was related to carbon chain length. Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12)to a maximum class 5 at C14, then reducing to class 3 at C16 & 18. In most cases the human scores were less those of the rabbits and reached a peak of class 3 with the C10 aclohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with hairless mouse skin. The response in guineapigs followed no obvious pattern and all scores were classed as <=3.

The results for C8, C12, C14, C16 and C18 alcohols have been given descriptive ratings for rabbits and man in various Iuclid datasets on aliphatic alcohols and these ratings together with the actual gradings from this reference are reported below.

1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol); reaction class 3 for rabbits and 2 for man (Kaestner 1977).
1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).

Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

Source: Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

Test condition: In this comparative study C4-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

Conclusion: This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible. This study is reported in Iuclid 2000.

Reliability: (2) valid with restrictions
Comparative study meeting generally accepted scientific principles.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Tetradecanol Cas# 112-72-1.

Kaestner, W. 1977. Zur Speziesabhangigkeit der Hautvertraglichkeit von Kosmetikgrundstoffen. J. Soc. Cos. Chem. 28: 741-754.

25-OCT-2005 (44) (45)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)</u>

Remark: Secondary reference by RTECS to data reported in Cutaneous Toxicity, proceedings of the 3rd Conference 1967. Drill & Lazar (eds). Academic Press, Inc. 1977. Not available.

Summary report indicates that 75 mg of the test substance was applied to human skin daily for 3 days producing a moderate skin reaction.

Source: RTECS, 2004
Hayes Consultancy Service Bromley, Kent

Test substance: Reported as 1-tetradecanol Cas # 112-72-1

Reliability: (4) not assignable
Secondary reference.

Reference: RTECS, 2004

25-OCT-2005 (57)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Remark: Report of unpublished reports from Henkel KGaA, TBD 860374 and 860375, originals unavailable.

The test substance was applied daily to rabbit skin on 4 consecutive days. Scoring according to Draize. Weak to sight skin reactions were observed after the first application, these did not intensify with subsequent appllications. Reaction described as slightly irritation.

Source: Hayes Consultancy Service Bromley, Kent

Test substance: > 95% 1-Tetradecanol (112-72-1). Samples of Lorol 14 tested obtained from Fa. Leciva, Prague.

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Tetradecanol Cas# 112-72-1.

25-OCT-2005 (44)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Remark: Secondary report of unpublished data from Henkel KGaA TBD 820011 and 820230 no 443. Original not available.

Test according to Directive 84/449/EEC, B4. Rabbit skin irritation described as slightly irritating, no further details provided.

Source: Hayes Consultancy Service Bromley, Kent

Test substance: > 95% 1-Tetradecanol (112-72-1)

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Tetradecanol Cas# 112-72-1.
25-OCT-2005 (44)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Remark: Secondary report of a study in hairless mice, unpublished report from Henkel KGaA TBD 760109 no 232.

The test substance was applied twice daily to the mouse skin and gently massaged into the skin. The number of treatment days was not reported. No further details available.

Result: described as not irritating.
Source: Hayes Consultancy Service Bromley, Kent
Test substance: > 95% 1-Tetradecanol (112-72-1)
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau Tetradecanol Cas# 112-72-1.
25-OCT-2005 (44)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Remark: Secondary report of a study in hairless mice, unpublished report from Henkel KGaA TBD 7820011 and 820230 no 443.

Applied to the skin of hariless mice. No other details available.

Result: described as slightly irritating.
Source: Hayes Consultancy Service Bromley, Kent
Test substance: > 95% 1-Tetradecanol (112-72-1)
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau Tetradecanol Cas# 112-72-1.
25-OCT-2005 (44)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Remark: Secondary report of unpublished data from Henkel KGaA R9601427. Original not available.

Application to human skin apparently to OECD guideline 404 was reported as being non-irritating. NO other details available.

Source: Hayes Consultancy Service Bromley, Kent
Test substance: > 95% 1-Tetradecanol (112-72-1)
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau
Tetradecanol Cas# 112-72-1.
25-OCT-2005 (44)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Species: other: New Zealand White rabbit
Exposure: Semiocclusive
Exposure Time: 4 hour(s)
No. of Animals: 3
Vehicle: water
PDII: 0
Result: not irritating
EC classificat.: not irritating

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1996
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: AVERAGE SCORE
- Erythema: Erythema (grade 1) observed at 1 hour after removal of dressings. All scores at other time points 0.
- Oedema: No oedema observed.

REVERSIBILITY: Initial erythema regressed in the first 24 hours. All scores at 24, 48 and 72 hours were 0.

OTHER EFFECTS: None reported.
Source: Sanders 1996b
Hayes Consultancy Service Bromley, Kent
Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: 2 male, 1 female
- Source: David Percival, Cheshire, UK
- Age: 12 -16 weeks
- Weight at study initiation: 2.36 - 2.54 kg
- Number of animals: 3

ADMINISTRATION/EXPOSURE
- Preparation of test substance: The test material was a white solid, the test site was moistened with 0.5 ml purified water

prior to application of 0.5 g of the solid.
- Area of exposure: 2.5 x 2.5 cm
- Occlusion: semi-occlusive
- Vehicle: None
- Total volume applied: 0.5 g
- Exposure period: 4 hours
- Postexposure period: 16 days
- Controls: Not rpeorted.
- Removal of test substance: Gentle swabbing with cotton.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours post application.

Test substance: Tradename Kalcol 6098
Conclusion: Following a 4 hour semi-occlusive exposure of Kalcol 6098 to rabbit skin there was no evidence of skin irritation between 24 and 72 hours after patch removal. Kalcol 6098 is not a skin irritant according to EU or GHs criteria.
Reliability: (1) valid without restriction
Guideline study.
Flag: Critical study for SIDS endpoint
Reference: Sanders, A. 1996b. Kalcol 6098: Acute dermal irritation test in the rabbit. SPL Project Number 140/496.
03-JAN-2006 (73)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Species: rabbit
Concentration: 50 %
Exposure: Occlusive
Exposure Time: 24 hour(s)
No. of Animals: 9
Vehicle: petrolatum
Result: slightly irritating

Method: other
Year: 1972
GLP: no
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Summary report of unpublished data submitted to CTFA in 1972. Test volume 0.1 ml (50% in petrolatum). The test substance produced minimal to slight irritation. The author reports that identical results were obtained in a similar study. This data is reported in other secondary references, Iuclid,

2000; Patty 2001,

Source: CIR, 1988
Hayes Consultancy Service Bromley, Kent

Reliability: (4) not assignable
Secondary reference.

Reference: Cosmetic Ingredient Review 1988 Final report on the safety assessment of cetearyl alcohol, cetyl alcohol, isostearyl alcohol, myristyl alcohol and behenyl alcohol. J. Am. Coll. Tox. 7(3): 359-413.

Iuclid 2000 European Commission - European Chemicals Bureau Hexadecan-1-ol Cas# 36653-82-4.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

25-JAN-2005 (16) (50) (67)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Remark: Secondary references to unpublished data reported in Patty 1963 cited by Opdyke, 1978, RTECS 2004 and Iuclid, 2000.

Guinea pig undiluted material produced only a mild effect.

Test substance: Cetyl alcohol, described in Patty, 1963 as a synthetic liquid C16 alcohol that may have contained impurities.

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Hexadecan-1-ol Cas# 36653-82-4.

Opdyke, D.L.J. 1978 Fragrance raw materials monographs Fd. Cos. Tox. 16: 683-686.

Patty, F.A (ed) 1963 Industrial Hygiene and Toxicology 2nd revised edition Vol. 11 Toxicology Chapter 34 Alcohols (J.F. Treon) Interscience publishers.

RTECS 2004 on-line 1-hexadecanol.

06-AUG-2005 (50) (66) (68) (70)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Remark: Unpublished data reported to CFTA 1976

Hexadecyl alcohol tested at 12% in petrolatum produced no irritation in human subjects (Epstein 1976).

Undiluted cetyl alcohol applied undiluted to intact and abraded rabbit skin in a 24 hour occlusive exposure was described as non-irritant (Levenstein, 1976).

Test substance: Hexadecanol

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Hexadecan-1-ol Cas# 36653-82-4

Opdyke, D.L.J. 1978 Fragrance raw materials monographs Fd. Cos. Tox. 16:683-686

25-JAN-2005 (50) (66)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Remark: Secondary report in RTECS and IUCLID 2000 of a human skin test in which 75 mg of test substance was applied to the skin for 3 days. the reaction is described as mild. The data was originally reported in Cutaneous Toxicity, Proceedings of the 3rd Conference 1976. Drill & Lazar (eds.)

Test substance: Hexadecanol

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Hexadecan-1-ol Cas# 36653-82-4.

RTECS 2004 on-line 1-hexadecanol.

18-JAN-2006 (50) (70)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Result: Cetyl alcohol gave a low irritancy score in the closed patch test regardless of concentration. An increase in degree of irritancy with concentration was seen using the nitrocellulose replica method.

Test condition: Comparison of two methods of assessing skin irritation in man using a group of 20 healthy volunteers (aged 26-29 years). Each test compound was adjusted to a molar concentration in the range 0.5 - 2 m.

Closed patch test: 15 ul of the test compound in petrolatum was applied to a filter disk fitted to a Finn chamber and applied to the skin of the upper back for 24 hours using Scanpor tape. The test site was scored visually for erythema at 1 and 24 hours after removal of the patch.

Nitrocellulose replica method: The test material was applied in petrolatum to the flexor side of ht eforearm using a semi-open 24 hour application. 30 minutes after removal a visual assessment was made and a replica of the skin surface was made using nitrocellulose disks. These disks were removed after 1-2 minutes and examined microscopically.

Test substance: Cetyl alcohol 96% pure, isomeric content not reported.

Reliability: (2) valid with restrictions
Comparative screening study, well documented, meets generally accepted scientific principles, acceptable for assessment.

Reference: Sato, A. et al. 1996. Evaluation of human skin irritation by carboxylic acids, alcohols, esters and aldehyde, with nitrocellulose-replica method and closed patch testing. Contact Dermatitis 34:12-16.

06-AUG-2005 (75)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Species	:	other: New Zealand White rabbit
Concentration	:	
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	3
PDII	:	0
Result	:	not irritating
EC classification	:	not irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1996
GLP	:	yes
Test substance	:	octadecanol (112-92-5)
Test substance	:	Tradename Kalcol 8098
Test condition	:	TEST ANIMALS: Rabbit - Strain: New Zealand White - Sex: Female - Source: David Percival Ltd, Cheshire, UK - Age: 12-16 weeks - Weight at study initiation: 2.56 - 2.73 kg - Number of animals: 3 ADMINISTRATION/EXPOSURE - Preparation of test substance: The test material was a white solid, the test site was moistened with 0.5 ml distlled water prior to application of 0.5 g of the solid. - Area of exposure: 2.5 x 2.5 cm

- Occlusion: semi-occlusive
- Vehicle: None
- Total volume applied: 0.5 g
- Exposure period: 4 hours
- Postexposure period: 72 hours
- Controls: None reported

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24, 48 and 72 hours post application

Result : The test material produced a primary irritation index of 0.0. No evidence of skin irritation was noted during the study, all scores were 0.

Conclusion : Following a 4 hour semi-occlusive exposure to rabbits skin Kalcol 8098 was non-irritating to rabbit skin.

Reliability : (1) valid without restriction
Guideline study

Source : Sanders 1996c
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Sanders, A. 1996c. Kalcol 8098: Acute dermal irritation test in the rabbit. SPL Project Number 140/502.

11.08.2005 (18)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Species: other: rabbit, guineapig, hairless mouse, human volunteers
Concentration: 50 %
Exposure: Occlusive
Exposure Time: 24 hour(s)
No. of Animals: 4
Vehicle: other: vaseline

Method: other
Year: 1977
GLP: no
Test substance: >= 90% 1-eicosanol (629-96-9)

Result: The most marked skin reactions were observed with rabbits, the degree of irritancy was related to carbon chain length.
Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12)to a maximum class 5 at C14, then reducing

to class 3 at C16 & 18. In most cases the human scores were less those of the rabbits and reached a peak of class 3 with the C10 aclohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with hairless mouse skin. The response in guineapigs followed no obvious pattern and all scores were classed as <=3.

The results for C8, C12, C14, C16 and C18 alcohols have been given descriptive ratings for rabbits and man in various Iuclid datasets on aliphatic alcohols and these ratings together with the actual gradings from this reference are reported below.

1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol); reaction class 3 for rabbits and 2 for man (Kaestner 1977).
1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).
Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

Source: Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

Test condition: In this comparative study C4-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

Conclusion: Icosanol produced minimal reversible irritation to rabbit skin

and was essentially non-irritating to human skin.
This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible.

Reliability: (2) valid with restrictions
Comparative study well documented, meets generally accepted scientific principles, acceptable for assessment but not for classification.

Reference: Kaestner, W. 1977. Zur Speziesabhangigkeit der Hautvertraglichkeit von Kosmetikgrundstoffen. J. Soc. Cos. Chem. 28: 741-754.

05-AUG-2005 (11)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Test substance: >= 90% 1-eicosanol (629-96-9)

Remark: Summary report of rabbit skin irritation test (OECD 404). The test material was reported as non-irritating.

Acute skin irritation/corrosion test (patch test) of Nacol 20 in the rabbit. Laboratory of Pharmacology & Toxicology, for Condea Chemie GmbH, 1986

Test substance: Tradename Nacol 20

Reliability: (4) not assignable
Secondary reference. (Study appears to be guideline and conducted at a contract laboratory but there are no experimental details to support this)

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Icosan-1-ol Cas# 629-96-9.

05-AUG-2005 (10)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Species: rabbit
Concentration: undiluted
Exposure: Semiocclusive
Exposure Time: 4 hour(s)
No. of Animals: 3
Vehicle: water
PDII: 0
Result: not irritating

EC classificat.: not irritating

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1997
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)
Result: The test material produced a primary irritation index of 0.0. No evidence of skin irritation was noted during the study other than very slight erythema at one test site at 1 hour after patch removal. All other scores were 0.
Source: Hempstock, 1997d
Hayes Consultancy Service Bromley, Kent
Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Female
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.81 - 3.15 kg
- Number of animals: 3

ADMINISTRATION/EXPOSURE
- Preparation of test substance: 0.5 g of the solid test material was moistened with 0.5 ml distlled water and applied to the shorn dorsal surface of the skin.
- Area of exposure: 2.5 x 2.5 cm
- Occlusion: semi-occlusive
- Vehicle: None
- Total volume applied: 0.5 g
- Exposure period: 4 hours
- Postexposure period: 72 hours
- Controls: None reported

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24, 48 and 72 hours post application

Test substance: Tradename Kalcol 220-80
Conclusion: Kalcol 220-80 is not a skin irritant when applied to rabbit skin undiluted in a 4 hour semi-occlusive exposure. Group mean 24+48+72 hours were 0.
Reliability: (1) valid without restriction
Guideline study.
Flag: Critical study for SIDS endpoint
Reference: Hempstock, C. 1997d. Kalcol 220-80: Acute dermal irritation test in the rabbit. SPL Project Number: 140/721.
06-AUG-2005 (13)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Remark: Secondary report from Condea Chemie GmbH reported in Iuclid 2000. Acute skin/irritation/corrosion test (patch test) of Nacol 22 RD in the rabbit. Laboratory of Pharmacology and Toxicology, 1986

Study to OECD guideline 404, no further details available. Nacol 22 RD was not irritating to rabbit skin.

Test substance: 1-docosanol (661-19-8) Tradename Nacol 22RD

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Docosan-1-ol Cas# 661-19-8.

06-AUG-2005 (17)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Species: other: rabbit, guineapig, hairless mouse, human volunteers
Concentration: 50 %
Exposure: Occlusive
Exposure Time: 24 hour(s)
No. of Animals: 4
Vehicle: other: vaseline

Method: other
Year: 1977
GLP: no
Test substance: >95% 1-docosanol (661-19-8)

Result: The most marked skin reactions were observed with rabbits, the degree of irritancy was related to carbon chain length. Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12)to a maximum class 5 at C14, then reducing to class 3 at C16 & 18. In most cases the human scores were less those of the rabbits and reached a peak of class 3 with the C10 aclohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with hairless mouse skin. The response in guineapigs followed no obvious pattern and all scores were classed as <=3.

The results for C8, C12, C14, C16 and C18 alcohols have been given descriptive ratings for rabbits and man in various Iuclid datasets on aliphatic alcohols and these ratings together with the actual gradings from this reference are reported below.

1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol); reaction class 3 for rabbits and 2 for man (Kaestner 1977).
1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).
Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

Source: Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

Test condition: In this comparative study C4-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

Conclusion: This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible.

Reliability: (2) valid with restrictions
Comparative study well documented, meets generally accepted scientific principles, acceptable for assessment but not for classification.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Docosan-1-ol Cas# 661-19-8.

Kaestner, W. 1977. Zur Speziesabhangigkeit der
Hautvertraglichkeit von Kosmetikgrundstoffen. J. Soc. Cos.
Chem. 28:741-754.
06-AUG-2005 (17) (18)

1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)

Test substance: 1-triacontanol (593-50-0)
Remark: Not a skin irritant in rabbits. No further details available.
Reliability: (4) not assignable
Reference: EPA (1983). US Environmental Protection Agency. Tolerances and Exemptions from Tolerances for Pesticide Chemical in or on Raw Agricultural Commodities: 1-Triacontanol. Fed. Reg. 48, (92), 21132.
05-APR-2007

5.2.2 Eye Irritation

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rabbit
Concentration	Undiluted
Dose	100 other: micro litre
Result	moderately irritating
Classification	Irritating
Method	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	1987
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Method: six New Zealand white rabbits, application of 100 microlitre into the lower conjunctival sac. Draize scoring criteria.

Result

Average scores	24hr	48hr	72hr
Conjunctivitis	2.50	2.61	2.06
Chemosis	1.67	1.17	0.83
Iritis	0.50	0.33	0.00
Corneal Opacity	1.00	1.50	1.00

Test substance	Test substance was neat ethanol.
Reliability	(2) valid with restrictions
Flag	Critical study for SIDS endpoint
Reference	Jacobs, GA, Guido, A. (1987) OECD eye irritation tests on three alcohols. J. Coll. Am. Toxicol. part A, 9, 56 - 57.
12.11.2004	(190)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rabbit
Concentration	100 % active substance
Number of animals	3
Vehicle	None
Result	moderately irritating
Classification	not irritating
Method	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	1998
GLP	Yes
Test substance	other TS: 100% ethanol

Method

The method was fundamentally OECD Guideline 405 with instillation of 0.1 ml, observation for 7 days and standard grading scales for lesions. However, a.Modified Maximum Average Score (MMAS) was derived by averaging the individual animal weighted scores at each time of observation and then selecting the highest (maximum) of these averages. This is a preferred result for this end point as it is a recent study carried out to a recognized protocol that is reported in detail.

Remark

Result

Average scores	Day 1	Day 2	Day 3
Corneal opacity	1.33	1.33	0.66
Iritis	0.33	0.66	0.33
Conjunctival redness	2.66	2.00	1.66
Chemosis	1.66	1.66	0.66

Individual animal observations reported. Full reversal of all symptoms in animals within 14 days. Most persistent effect conjunctival redness, still present, grade 1, at 7 days (last observation time before 14 day observation.)

Test substance	Concentration undiluted/100%
Reliability	(2) valid with restrictions
Flag	Critical study for SIDS endpoint
Reference	ECETOC Eye Irritation Databank (2nd ed), TR48(2) 1998.
12.11.2004	(191)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	other: human, rabbit
Concentration	
Dose	
Exposure time	
Comment	other: review of published work
Method	
Year	1986
GLP	

	other TS
Remark	Routes include direct contact with and without anesthesia, vapour exposure, injection into orbit, acute and chronic alcohol intoxication and fetal alcohol syndrome.
Test substance	spirits, toiliery solutions; various concentrations alcohol 1.
Conclusion	Splashes of alcoholic spirit (20-50% alcohol causes stinging discomfort and reflex closure with no lastic effects. 2. On rabbit cornea, 50% alcohol causes mild reaction graded 20 on a scale of 100. 3. repeated applicatuon of 7 drops of 40 to 80% alcohol caused loss of corneal epithelium and endothelium followed by haemorrhage into conjunctiva, inflitration and vascularization of corneal stroma. 4. Shaving lotions etc may contain up to 90% alcohol; severe reactions with slow recovery may occur, possibly due to other components. 5. High vapour concentrations may cause stinging and watering of eyes above 0.25%. By other routes - ocular effects are not irritation.
Reliability	(4) not assignable
Flag	Critical study for SIDS endpoint
Reference	Grant, W.M. Toxicology of the eye. Edn 3. (1986). Charles C Thomas, Springfield, USA.
12.11.2004	(192)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rabbit
Result	not irritating
Classification	not irritating
Method	OECD Guideline 405 "Acute Eye Irritation/Corrosion"
Year	1983
GLP	No
Test substance	ethanol (64-17-5)
Test substance	Pure ethanol
Reliability	(4) not assignable
Reference	BASF AG Toxicology Department unpublished Research (83/64) 06-07-1983.
12.11.2004	(193)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rabbit

Result	not irritating
Classification	
Method	other
Year	1979
GLP	No
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	After Fed Reg vol 38 no. 18727-09-1973
Reliability	(4) not assignable
Reference	BASF AG Toxicology Department Unpublished research (78/810) 04-09-1979.
12.11.2004	(194)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rabbit
Result	moderately irritating
Classification	
Method	Draize Test
Year	1978
GLP	No
Test substance	ethanol (64-17-5)
Test Substance	96% ethanol.
Reliability	(4) not assignable
Reference	BASF AG Toxicology Department Unpublished research TNO Report No. R5724 (1978).
12.11.2004	(195)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance:	1-butanol
Test species/strain:	Rabbit
Test method:	Not Stated
GLP:	No
Test results:	When 1.62 or 20 mg BA was instilled into rabbit eyes, severe eye irritation occurred after 72 and 24 hours, respectively.
Comments:	
Reference:	US DHEW. 1978. Registry of toxic effects of chemicals, Washington DC, US Department of Health, Education and Welfare. As cited in World Health Organization (WHO). 1987. Environmental Health Criteria 65: Butanols - Four Isomers: 1-Butanol, 2-Butanol, tert-Butanol, Isobutanol. WHO. Registry of Toxic Effects of Chemical Substances.p.1301, 1985-86.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-butanol
Test species/strain: Rabbit
Test method: Not Stated
GLP: No

Test results: When 0.005 ml BA was instilled into rabbit eyes, severe corneal irritation resulted.
Comments:
Reference: Patty, F.A. 1982.Industrial hygiene and toxicology, 3 rd ed., New York, Chichester, Brisbane, Toronto, Singapore, WileyInterscience. IIC: 4571-4578. As cited in World Health Organization (WHO). 1987. Environmental Health Criteria 65: Butanols - Four Isomers: 1-Butanol 2-Butanol tert-Butanol Isobutanol. WHO.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-butanol
Test species/strain: Humans
Test method: Sixteen subjects were exposed (i.e. eye only) to n-butanol at concentrations up to 300 mg/m 3 (990 ppm) for up to an hour, three times daily on 5 different days. Ratings of ocular irritation intensity were. obtained continuously during all 3 runs.
Test results: During run 2, the authors observed a slight increase in perceived eye irritation intensity for all exposure concentrations. However, the threshold for irritation (conjunctival hyperemia) was never clearly exceeded.

GLP: No
Comments:
Reference: Hempel-Jorgensen, A., Hudnell, H.K., Kjaergaard, S.K., and Molhave, L 1999. Time Course of Sensory Eye Irritation in Humans Exposed to n-Butanol and 1-octene.Arch. Environ. Health 54(2), 86-94.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: rabbit
Concentration: undiluted
Dose: .1 ml
Comment: not rinsed
No. of Animals: 6
Vehicle: other: undiluted
Result: irritating
EC classificat.: irritating

Method: other: contract laboratory procedure
Year: 1977
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: AVERAGE SCORE: The scores were reported as prescribed by the FDA 1965. Although individual animal data was provided only the converted scores were reported so it is not possible to present the data according to EC/GHS criteria. The average score (includes all end points) for each tiem point was as follows:

1 hour: 14
24 hours: 31.8
48 hours: 37.7
72 hours: 32.4

DESCRIPTION OF LESIONS:
- Cornea: opacity (slight density and involving about half the corneal surface) in all rabbits from 24 hours after instillation. At 72 hours described as easily discernable to opalescent and involving about 1/4 to 3/4 of the corneal surface in 5/6.
- Iris: barely perceptible to minimal iritis (grade 1) in 4/6 rabbits from 24 hours after instillation. At 72 hours described as barely perceptible to slight in 3/6.
- Conjunctivae (Redness): Slight to severe conjunctivitis in all eyes from 24 hours. At 72 hours described as slight to severe in 6/6.
- Conjunctivae (Chemosis): Moderate to pronounced chemosis of the eye lids with a slight to copious watery-mucoid discharge in all animals.

REVERSIBILITY: Irritation was evident up to and including the 72 hour observation period. There was improvement in one animal, little change in 3 animals and a worsening of the condition in 2.

Source: Scientific Associates, Inc. 1977c
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6

- Controls: The other eye served as control.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 72 hours

EXAMINATIONS
- Ophthalmoscopic examination: Not reported
- Scoring system: FDA 1965
- Observation period: 1, 24, 48 and 72 hours.
- Tool used to assess score: Fluorescein

Test substance: Tradename Alfol 6.
Conclusion: Based on the descriptions of the lesions it is considered that Alfol 6 is classifiable as an irritant according to EU criteria and a class 2 irritant according to GHS.
Reliability: (2) valid with restrictions
Reasonably documented, however the test was terminated at 72 hours when there was still marked irritation.
Flag: Critical study for SIDS endpoint
Reference: Scientific Associates, Inc. 1977c. Acute oral toxicity (LD50) in rats; Acute dermal toxicity (LD50) in rabbits, Dermal irritation test in rabbits; Eye irritation test in rabbits; Inhalation toxicity tests in rats: ALFOL 6. S.A. Number 233619.
11-NOV-2004 (62)

<u>1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)</u>

Species: rabbit
Concentration: undiluted
Dose: .1 ml
Comment: not rinsed
No. of Animals: 4
Vehicle: none
Result: irritating

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1987
GLP: yes
Test substance: >95% 1-hexanol (111-27-3)

Result: AVERAGE SCORE (24+48+72 hour)
- Cornea: Individual 3, 2, 2, 1.7 Mean 2.2
- Iris: Individual 2, 1, 1, 1.3 Mean 1.3

- Conjunctivae (Redness): Individual 3, 2, 3, 2.7 Mean 2.7
- Conjunctivae (Chemosis): Individual 3, 2, 3, 2 Mean 2.5
- Overall irritation score: MMAS (modified maximum score 64.8)

REVERSIBILITY: Effects on the cornea and iris had reversed by 7 days, redness and/or chemosis persisted to 7 days in one rabbits, 10 days in 2 animals and 14 days in the final rabbit, all scores were 0 by day 21.

Source: ECETOC, 1998

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Unspecified
- Source: No data

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Postexposure period: 21 days

EXAMINATIONS
- Ophthalmoscopic examination: No data
- Scoring system: No data
- Observation period: 24, 48, 72 hours, 7, 10, 14 and 21 days (assessments made until the test eye for each animal showed complete reversal to normal up to 21 days)
- Tool used to assess score: No data

The study was included as part of a data base of in vivo eye irritation results. All studies were conducted to OECD guideline 405 under GLP.

Conclusion: 1-hexanol is classifiable as an eye irritant according to EU criteria (based on 24+48+72 hour mean scores =>2 for corneal opacity (2.2) and chemosis (2.5) and =>2.5 for conjunctival redness (2.7) reversible within 21 days. According to GHS criteria 1-hexanol is a Class 2A irritant based on individual mean 24+48+72 hour scores in at least 2 test animals of => 1 for corneal opacity and iritis and => 2 in at least 2 test animals for conjunctival chemosis and redness. Only 1 animal scored => 3 for corneal opacity or => 1.5 for iritis.

Reliability: (1) valid without restriction
Guideline study

Flag: Critical study for SIDS endpoint

Reference: ECETOC 1998 Eye irritation reference chemicals data bank (second edition). ECETOC Technical report No. 48(2).

15-JUL-2005 (20)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: rabbit
Concentration: undiluted
Comment: not rinsed
No. of Animals: 6
Vehicle: other: undiluted
Result: irritating
EC classificat.: irritating

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1987
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: AVERAGE SCORE (24+48+72 hour)
- Cornea: 1.3 (96 hr 2) (opacity)
- Iris: 0.1 (96 hr 0)
- Conjunctivae (Redness): 2.5 (96 hr 1.8)
- Conjunctivae (Chemosis): 0.8 (96 hr 0)

Individual animal data were not provided.

DESCRIPTION OF LESIONS: Scores only reported no description of lesions.

REVERSIBILITY: Effects had not fully reversed over the observation period. Corneal opacity increased up to 24 hours. All other parmeters scored showed a reduction in response over 96 hours.

OTHER EFFECTS: The % surface of the cornea affected by corneal damage was reported as follows: 4 hour 77%; 24 hours 67%; 48 hour 50%; 72 hour 17%; 96 hours 0%.

Source: Jacobs & Martens, 1987
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted

- Amount of substance instilled: 0.1 ml
- Vehicle: undiluted
- Postexposure period: 96 hours

EXAMINATIONS
- Ophthalmoscopic examination: Not reported
- Scoring system: Draize scores at 4, 24, 48, 72 and 96 hours post exposure.
- Observation period: 96 hours
- Tool used to assess score: One drop 2% sodium fluorescein .

Conclusion: 1-hexanol is an eye irritant according to EU criteria with group mean 24+48+72 hour scores for conjunctival redness of 2.5. Although individual scores are not available, 6 animals were used and it is considered that 1-hexanol is a Class 2A eye irritant according to GHS criteria.
Reliability: (2) valid with restrictions
Guideline study without detailed documentation.
Flag: Critical study for SIDS endpoint
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3.

Jacobs, G.A. & Martens, M.A., 1987 Skin and eye irritation tests on hexanol. J. Am .Coll. Toxicol. Acute Toxicity Data 11(6): 722.
15-JUL-2005 (29) (30)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Remark: Iuclid 2000 reports (in summary) 2 eye irritation studies in rabbits with Alfol 6. Both tests are described as Draize tests. The EC classification was given as irritating in both tests although in one test the result was described as highly irritating (Scientific Assoc. 1965 for Continental Oil) and in the other moderately irritating (Hazelton Inc. 1982 for Conoco Inc). No further details are available.
Test substance: 1-hexanol (111-27-3) Trade name Alfol 6
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3.
11-NOV-2004 (29)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Remark: A summary report of a rabbit eye irritation test carried out

to OECD 405 on Nacol 6 RD for Condea Chimie GmbH in 1986. The result is given as moderately irritating with an EC classification of irritating. No further details are available.

Test substance: 1-hexanol (111-27-3) Tradename Nacol 6 RD
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3.
11-NOV-2004 (29)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Remark: Data cited in Iuclid 2000.
Test substance: Reported as hexanol 98%
Reliability: (4) not assignable
Reference: ECETOC, 1992 Eye irritation, chemicals reference data bank. Technical Report No. 48.

Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3.
17-OCT-2004 (21) (29)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Species: rabbit
Concentration: undiluted
Dose: .1 ml
Comment: not rinsed
No. of Animals: 3
Vehicle: none
Result: irritating
EC classificat.: risk of serious damage to eyes

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1987
GLP: yes
Test substance: > 90% 1-octanol (111-87-5)

Result: AVERAGE SCORE (24+48+72 hr mean)
- Cornea: Individual scores 2, 1, 1 (group mean 1.33)
- Iris: All 1 (group mean 1)
- Conjuntivae (Redness): 2.3, 1.7, 1.3 (group mean 1.8)
- Conjuntivae (Chemosis): 1, 1.3, 0.7 (group mean 1)

DESCRIPTION OF LESIONS: Iritis, slight to moderate

conjuncitivitis and areas of very slight/slight corneal opacity during the first 72 hours. Very slight conjunctivitis observed in all 3 animals at days 8 and 15.

REVERSIBILITY: Very slight conjunctivitis persisted in 2 animals until termination on day 22. Iritis persisted in one of these rabbits until day 22.

OTHER EFFECTS: Blepharitis of the lower lid seen in 2 rabbits at 72 hours persisting to day 8 in one rabbit. Very slight/slight initial pain response.

Source: Johnson 1996d
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: female
- Source: Froxfield SPF Rabbits, Hampshire, UK
- Age: 5 months
- Weight at study initiation: 2.88 - 3.13 kg
- Number of animals: 3
- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 22 days

EXAMINATIONS
- Scoring system: As prescribed in OECD test method.
- Observation period: 22 days
- Tool used to assess score: Ophthalmoscope or pencil beam tourch. Fluorescein used from 24 hours onward as required to aid corneal examination.

Test substance: Tradename Kalcol 0898

Conclusion: Kalcol 0898 is an eye irritant according to EU criteria based on individual mean 24+48+72 hour scores for iritis of >= 1 in all test animals. This material is considered a category 1 eye irritant under GHS and to cause a risk of serious damage to eyes (EU) based on persistence of iritis (1 rabbit) and conjunctivitis (2 rabbits) to 22 days.

Reliability: (1) valid without restriction
Guideline study

Flag: Critical study for SIDS endpoint

Reference: Johnson, I.R. 1996d. Kalcohl 0898: Acute eye irritation test in the rabbit. Final report. Report No. 96/KAS215/0676.

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Species: rabbit
Concentration: undiluted
Dose: .1 ml
Comment: not rinsed
No. of Animals: 3
Vehicle: none
Result: irritating

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1987
GLP: yes
Test substance: > 90% 1-octanol (111-87-5)
Result: AVERAGE SCORE (24+48+72 hour)
- Cornea: Individual 1, 2, 2 Mean 1.7
- Iris: Individual 0, 1, 1 Mean 0.7
- Conjunctivae (Redness): Individual 1.7, 2.3, 2.7 Mean 2.2
- Conjunctivae (Chemosis): Individual 1.7, 3, 2.7 Mean 2.5
- Overall irritation score: MMAS (modified maximum average score) 41.0

REVERSIBILITY: Complete reversal in 14 days for all 3 test animals, 1 eye appeared normal after 7 days.
Source: ECETOC, 1998
Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Unspecified
- Source: No data

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Postexposure period: 21 days

EXAMINATIONS
- Ophthalmoscopic examination: No data
- Scoring system: No data
- Observation period: 1, 24, 48, 72 hours, 7, 10, 14 and 21 days (assessments made until the test eye for each animal showed complete reversal to normal up to 21 days)
- Tool used to assess score: No data

The study was included as part of a data base of in vivo eye

irritation results. All studies were conducted to OECD guideline under GLP.

Conclusion: 1-octanol is classifiable as an eye irritant based on scores of =>2 for corneal opacity, =>1 for iritis and =>2 for chemosis. The lesions were reversible within 14 days. According to GHS criteria 1-hexanol is a Class 2A irritant based on individual mean 24+48+72 hour scores in at least 2 test animals of => 1 for corneal opacity and iritis and => 2 in at least 2 test animals for conjunctival chemosis and redness.

Reliability: (1) valid without restriction
Guideline study.

Flag: Critical study for SIDS endpoint

Reference: ECETOC 1998 Eye irritation reference chemicals data bank (second edition). ECETOC Technical report No. 48(2).

16-JUL-2005 (39)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Species: other: New Zealand White albino rabbits
Concentration: undiluted
Dose: .1 ml
Comment: not rinsed
No. of Animals: 6
Vehicle: none
Result: irritating
EC classificat.: irritating

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1987
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Result: AVERAGE SCORE mean 24+48+72hr (96 hour mean)
- Cornea: 2.23 (2)
- Iris: 0.7 (0.5)
- Conjuntivae (Redness): 2.57 (2)
- Conjuntivae (Chemosis): 1.9 (1)

Individual scores were not reported.

DESCRIPTION OF LESIONS: none given.

REVERSIBILITY: The observation period was 96 hours. At this time point mean scores had reduced for all parameters as indicated in parentheses above.

OTHER EFFECTS: The mean surface of corneal damage was reported this was at a maximum of 75% at 24 hours reducing to 5% at 96 hours.

Source: Jacobs 1987
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: rabbits
- Strain: New Zealand White
- Sex: no data
- Source: no data
- Number of animals: 6
- Controls: no

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 96 hours

EXAMINATIONS
- Ophthalmoscopic examination:
- Scoring system: Draize
- Observation period: 96 hours
- Tool used to assess score: 2% sodium fluorescein before visual scoring of % corneal damage

Conclusion: 1-octanol is an eye irritant according to EU criteria based on a mean 24+48+72 hour score for 6 rabbits of 2.57 for conjuctivitis and 2.23 for corneal opacity. Results are only given up to 96 hours post instillation but the evidence was that the effects were reversing at this time point. Lack of individual scores precludes accurate assessment by GHS however based on the mean scores of 6 rabbits for corneal opacity of 2.23 and for iritis of 0.7 and given the evidence of reversibility 1-octanol is considered a Category 2A eye irritant.

Cited in Iuclid 2000 and Patty 2001.

Reliability: (2) valid with restrictions
Guideline study without detailed information.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Octan-1-ol Cas# 111-87-5.

Jacobs, G.A. 1987. OECD eye irritation test on 1-octanol. Institute of Hygiene and Epidemiology 726.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols
(Monohydric alcohols) John Wiley & Sons - on line.
11-NOV-2004 (62) (66) (90)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Species: rabbit
Concentration: undiluted
Dose: .1 ml
Comment: not rinsed
No. of Animals: 3
Vehicle: none
Result: moderately irritating
EC classificat.: not irritating

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1996
GLP: yes
Test substance: > 90% 1-decanol (112-30-1)

Result: AVERAGE SCORE (24+48+72 hour)
- Cornea: individual scores 2, 1. 0.7 (group mean score 1.23)
- Iris: individual scores 0.7, 0.3, 0.7 (group mean score 0.56)
- Conjunctivae (Redness): 2.7, 1.3. 1.3 (group mean score 1.77)
- Conjunctivae (Chemosis): individual scores 1.3, 0.3, 0.3 (group mean score 0.63)

DESCRIPTION OF LESIONS: Slight or moderate conjunctivitis, very slight or slight corneal opacity and iritis were seen in all animals during the first 48 hours following instillation. On Day 4, all animals still showed slight conjunctivitis and one showed a small area of slight corneal opacity.

REVERSIBILITY: Slight conjunctivitis persisted in one rabbit to Day 8 and in another to Day 15. All scores 0 by day 22.

OTHER EFFECTS: Instillation of the test material caused a very slight initial pain response.

Source: Johnson 1996e
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: female
- Source: Froxfield SPF Rabbits, Hampshire, UK

- Age: 5 months
- Weight at study initiation: 2.63 - 2.99 kg
- Number of animals: 3
- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 22 days

EXAMINATIONS
- Scoring system: As prescribed in OECD test method.
- Observation period: 22 days
- Tool used to assess score: Ophthalmoscope or pencil beam torch. Fluorescein used from 24 hours onward as required to aid corneal examination.

Test substance: Tradename Kalcohl 1095
Conclusion: Kalcol 1095 is not an eye irritant according to EU criteria. Using GHS criteria Kalcol 1095 is an irritant category 2A based on scores for corneal opacity >= 1 in 2 rabbits and persistence >7 and <22 days.
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
Reference: Johnson, I.R. 1996e. Kalcohl 1095: Acute eye irritation test in the rabbit. Final report. Report No. 96/KAS221/0715.
05-AUG-2005 (57)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Test substance: > 90% 1-decanol (112-30-1)
Remark: Secondary report from unobtainable Russian language reference. Corneal injury was reported following instillation of decanol into the eyes of rabbits. No further details available.
Reliability: (4) not assignable
Secondary reference.
Reference: Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.
26-OCT-2004 (70)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Remark: Secondary report from unobtainable Russian reference. 500 mg Decanol applied to the rabbit eye produced mild irritation.
Reliability: (4) not assignable

Secondary reference, original unavailable.
Reference: RTECS on line 2004 Decyl Alcohol.
08-OCT-2004 (74)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Species	:	other: New Zealand White rabbit
Concentration	:	undiluted
Dose	:	.1 ml
Exposure Time	:	
Comment	:	not rinsed
Number of animals	:	3
Result	:	not irritating
EC classification	:	not irritating
Method	:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	:	1996
GLP	:	yes
Test substance	:	dodecanol (112-53-8)
Test substance	:	Tradename Kalcol 2098
Test condition	:	TEST ANIMALS: Rabbit - Strain: New Zealand White - Sex: male - Source: David Percival Ltd, Cheshire, UK - Age: 12-16 weeks - Weight at study initiation: 2.5-2.87 kg - Number of animals: 3 - Controls: Untreated eye used as control ADMINISTRATION/EXPOSURE - Preparation of test substance: the substance was a solid and was warmed in a warming bath to 40C prior to instillation. - Amount of substance instilled: 0.1 ml - Vehicle: None - Postexposure period: 72 hours EXAMINATIONS - Scoring system: Draize adn modifies Kay and Callandra. - Observation period: 72 hours - Tool used to assess score: Standard ophthalmoscope.
Result	:	AVERAGE SCORE (24+48+72 hour) - Cornea: All 0 - Iris: All 0 - Conjunctivae (Redness): Individual scores 2 rabbits 0 the remaining

rabbit 0.3. (group mean score 0.1)
- Conjunctivae (Chemosis): All 0
- Overall irritation score: maximum group mean score of 8.7. Classified as a minimal eye irritant according to Kay & Callandra (modified).

DESCRIPTION OF LESIONS: No corneal or iridial effects were noted suring the study. Moderate conjunctival irritation was noted in two treated eyes with minimal conjunctival irritation in the remaining treated eye one hour after treatment. Minimal conjunctival redness was noted in one treated eye at the 24 hour observation point.

REVERSIBILITY: All scores were 0 at 48 and 72 hours.

OTHER EFFECTS: Conjunctival discharge was noted in all animals one hour after instillation.

Conclusion : Kalcol 2098 is not irritating to the rabbit eye using either EU or GHS criteria.

Reliability : (1) valid without restriction
Guideline study

Source : Sanders 1996d
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.

11.08.2005 (20)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Species: other: New Zealand White rabbit
Concentration: undiluted
Dose: .1 ml
Comment: not rinsed
No. of Animals: 3
Vehicle: none
Result: moderately irritating
EC classificat.: not irritating

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1987
GLP: yes
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: AVERAGE SCORE (24+48+72 hour)

- Cornea: Individual scores 0, 1, 1 (group mean 0.7)
- Iris: individual scores 0, 1, 0.3 (group mean score 0.43)
- Conjunctivae (Redness): Individual scores 0.7, 2, 1.7 (group mean score 1.47)
- Conjunctivae (Chemosis): Individual scores 0.3, 1.7, 1.7 (group mean score 1.23)
- Overall irritation score: Maximum group mean score 27.3 at 24 hours.

The substance is classified as a moderate irritant according to Kay and Callandra.

DESCRIPTION OF LESIONS: Diffuse corneal opacity was noted in 2 treated eyes at the 24, 48, and 72 hour observations.
Iridial inflammation was noted in 2 treated eyes at the 24 hour observation and persisted in 1 treated eye at the 48 and 72 hour observations.
Moderate conjunctival irritation was noted in all treated eyes 1 hour after treatment and persisted in 2 treated eyes at the 24 and 48 hour observations. Minimal conjunctival irritation was noted in 1 treated eye at the 24 and 48 hour observations and in 2 treated eyes at the 72 hour and 7 day observation.

REVERSIBILITY: All corneal and iridial scores and scores for conjunctival chemosis were normal by day 7. Conjunctival redness persisted in 2 rabbits through day 7 but scores were 0 by day 14. The effects were therefore fully reversible.

OTHER EFFECTS: Discharge was observed from all treated eyes 1 hour after instillation and persisted in one eye for 48 hours and in another for 72 hours. All eyes were clear at 7 days.

Source: Sanders 1996f
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: male
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.67-2.94 kg
- Number of animals: 3
- Controls: Untreated eye used as control

ADMINISTRATION/EXPOSURE
- Preparation of test substance: the substance was a solid and

was ground to a fine powder prior to instillation. Measured using an adapted syringe.
- Amount of substance instilled: 0.1 ml (ca 46 mg)
- Vehicle: None
- Postexposure period: 14 days

EXAMINATIONS
- Scoring system: Draize and modified Kay and Callandra.
- Observation period: 14 days
- Tool used to assess score: Standard ophthalmoscope.

Test substance: Tradename Kalcol 4098.
Conclusion: Kalcol 4098 applied as a powder is not classifiable as an eye irritant according to EU criteria. Kalcol 4098 is however a category 2A eye irritant according to GHS criteria based on corneal opacity of >= 1 in 2 test animals and persistence beyond 7 days. Effects were fully reversible by day 14.
Reliability: (1) valid without restriction
Guideline study.
Flag: Critical study for SIDS endpoint
Reference: Sanders, A. 1996f. Kalcol 4098: Acute eye irritation test in the rabbit. SPL Project Number 140/596.
16-OCT-2004 (60)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Species: other: New Zealand White rabbit
Concentration: 10 %
Dose: .1 ml
Comment: not rinsed
No. of Animals: 3
Vehicle: other: polyethylene glycol 400
Result: not irritating
EC classificat.: not irritating

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1997
GLP: yes
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): Individual scores 0.3, 0.3, 0 (group mean score 0.2)
- Conjunctivae (Chemosis): 0. 0, 0.3 (group mean score 0.1)
- Overall irritation score: maximum group mean score 8.7 at 1

hour post instillation. Described as a minimal eye irritant according to modified Kay & Calandra.
DESCRIPTION OF LESIONS: At 1 hour post instillation Grade 2 redness of the conjunctival membrane was noted in 2 treated eyes with grade 1 redness of the conjunctival membrane noted in the remaining treated eye. Conjunctival redness (grade 1) persisted in in 2 treated eyes at the 24 hour observation. Chemosis was also observed in all eyes at 1 hour post instillation (grade1 and 2) persisting in one treaed eye until 24 hours. Grade 3 discharge was noted in 1 treated eye with grade 1 noted in one other treated eye at the 1 hour observation. No other evidence of eye irritation was noted during the study.

REVERSIBILITY: All treated eyes appeared normal 48 and 72 hours after instillation.

OTHER EFFECTS:

Source: Hempstock 1997b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: male
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.56-2.80 kg
- Number of animals: 3
- Controls: Untreated eye used as control

ADMINISTRATION/EXPOSURE
- Preparation of test substance: the substance was prepared as a 10% solution in polyethylene glycol 400,
- Amount of substance instilled: 0.1 ml
- Vehicle: polyethylene glycol 400
- Postexposure period: 72 hours

EXAMINATIONS
- Scoring system: Draize and modified Kay and Calandra.
- Observation period: 72 hours
- Tool used to assess score: Standard ophthalmoscope.

Test substance: Tradename Kalcol 4098.

Conclusion: When instilled into the rabbit eye as a 10% solution in polyethylene glycol 400, Kalcol 4098 was not classified as an eye irritant by either EU of GHS criteria.

Reliability: (1) valid without restriction
Guideline study.
Reference: Hempstock, C. 1997b. Kalcol 4098 (10%): Acute eye irritation test in the rabbit. SPL Project Number 140/780R.
16-OCT-2004 (23)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Species: rabbit
Concentration: 100 mg
Exposure Time: 24 hour(s)
Comment: rinsed after (see exposure time)
No. of Animals: 6
Vehicle: other: applied as solid
Result: not irritating
EC classificat.: not irritating

Method: other: contract laboratory protocol
Year: 1997
GLP: no data
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: AVERAGE SCORE: The scores were reported as prescribed by the FDA 1965. Although individual animal data was provided only the converted scores were reported so it is not possible to present the data according to EC/GHS criteria. The average score (includes all end points) for each time point was as follows:

1 hour: 6.7
24 hours: 18
48 hours: 12.5
72 hours: 6

DESCRIPTION OF LESIONS:
- Cornea: opacity slight to easily discernible involving 1/4 to 3/4 of the corneal surface observed in all animals. At 72 hours there was no corneal involvement in any animal.
- Iris: barely perceptible to minimal iritis (grade 1) in 1/6 rabbits at 24 hours after instillation. No iritis at 48 or 72 hours.
- Conjunctivae (Redness): Slight to moderate conjuctivitis in all eyes from 24 hours. At 72 hours there was minimal to slight redness in 6/6.
- Conjunctivae (Chemosis): Minimal to pronounced chemosis of the eye lids with a slight watery-mucoid discharge in all

animals. At 72 hours barely perceptible to moderate chemosis 4/6 and slight discharge 2/6.

REVERSIBILITY: There was a gradual improvement in all animals. By the end of the 72 hour observation period there was no involvement of the iris or cornea. Minimal to slight redness and barely perceptible to moderate chemosis were still evident.

Source: Scientific Associates, Inc. 1977b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6
- Controls: The other eye served as control.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: applied as a solid
- Amount of substance instilled: 100 mg
- Vehicle: none
- Postexposure period: 72 hours
- Rinsing: The treated eyes were rinsed after 24 hours to remove residual test material.

EXAMINATIONS
- Ophthalmoscopic examination: Not reported
- Scoring system: FDA 1965
- Observation period: 1, 24, 48 and 72 hours.
- Tool used to assess score: Fluorescein

Test substance: Tradename Alfol 14.

Conclusion: Based on the description of the lesions and the consistent reduction of severity of the effects over the 72 hours observation period it is considered that Alfol 14 is not classifiable as an eye irritant according to EU or GHS criteria.

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: Scientific Associates, Inc. 1977b. Acute oral toxcity (LD50) in rats, acute dermal toxicity (LD50) in rabbits,

dermal irritation test in rabbits, eye irritation test in rabbits, and inhalation toxicity test in rats. ALFOL 14 alcohol.
12-OCT-2005 (64)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Species: rabbit
Concentration: 50 %
No. of Animals: 2
Vehicle: no data
Result: slightly irritating

Method: other: not specified
GLP: no
Test substance: other TS: C14 myristic alcohol

Remark: Summary report of unpublished Henkel data (Potokar Archive No. 232). No details of method except that 50 ul of 50% myristic alcohol was instilled. Slight conjunctival redness was reported up to 6 hours after instillation. There was no involvement of cornea or iris. Irritant response described as slight.

There is an entry in Iuclid 2000 describing slight eye irritation using the Draize method, this appears to be the same study as above as it refers to the same Henkel report.
Source: Iuclid 2000, Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau Tetradecanol Cas# 112-72-1.
16-JUL-2005 (44)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Species: other: New Zealand White rabbit
Concentration: undiluted
Dose: .1 ml
Comment: not rinsed
No. of Animals: 3
Vehicle: none
Result: not irritating
EC classificat.: not irritating

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1996
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: AVERAGE SCORE (24+48+72 hour)
- Cornea: individual scores 0.3, 0, 0 (group mean score 0.1)
- Iris: 0
- Conjunctivae (Redness): All 0.3 (group mean score 0.3)
- Conjunctivae (Chemosis): 0, 0.3, 0.3 (group mean score 0.2)
- Overall irritation score: Maximum group mean score 15.3 at 1 hour post instillation. Classified as a mild irritant according to a modified Kay and Calandra system.

DESCRIPTION OF LESIONS: Dulling of the cornea noted in 2 animals 1 hour after instillation, diffuse corneal opacity noted in 1 rabbit at 24 hours post instillation. Iridial inflammation noted in 2 animals at 1 hour post instillation only. Moderate conjunctival irritation noted in all eyes at 1 hour which reduced to minimal conjunctival irritation at 24 hours.

REVERSIBILITY: All eyes were normal at 48 and 72 hours post instillation.

OTHER EFFECTS: Residual test material noted around the treated eyes at 1 hour post instillation.

Source: Sanders 1996g
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: male
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.69-3.01 kg
- Number of animals: 3
- Controls: Untreated eye used as control

ADMINISTRATION/EXPOSURE
- Preparation of test substance: White granular solid applied using an adapted syringe.
- Amount of substance instilled: 0.1 ml (ca 78 mg)
- Vehicle: None
- Postexposure period: 72 hours

EXAMINATIONS
- Scoring system: Draize and modified Kay and Callandra.
- Observation period: 72 hours
- Tool used to assess score: Standard ophthalmoscope.

Test substance: Tradename Kalcol 6098
Conclusion: Kalcol 6098 is not an eye irritant according to EU or GHS criteria.
Reliability: (1) valid without restriction
Guideline study.
Flag: Critical study for SIDS endpoint
Reference: Sanders, A. 1996g. Kalcol 6098: Acute eye irritation test in the rabbit. SPL Project Number 140/498.
03-JAN-2006 (74)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Species: rabbit
Concentration: undiluted
Dose: .1 ml
Comment: no data
No. of Animals: 6
Vehicle: none
Result: not irritating

Method: Draize Test
Year: 1959
GLP: no data
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: Report of 2 similar unpublished studies carried out according to the Draize method 1959. Ocular irritation was scored at 1,2,3,4 and 7 days post instillation. An average score of 1 was reported on day 1 post instillation and signs of ocular irritation had cleared by day 2. In a second similar study the average score at day 1 was again 1 and all signs of irritation had cleared by day 2. Cetyl alcohol was considered at most minimally irritating in these tests. This study also appears to be reported in Iuclid 2000 and Patty, 2001.
Test substance: Cetyl alcohol (hexadecanol) isomer content not reported)
Reliability: (4) not assignable
Secondary reference some experimental detail provided.
Reference: Cosmetic Ingredient Review 1988 Final report on the safety assessment of cetearyl alcohol, cetyl alcohol, isostearyl alcohol, myristyl alcohol and behenyl alcohol. J. Am. Coll. Tox. 7(3):359-413

Iuclid 2000 European Commission - European Chemicals Bureau
Hexadecan-1-ol Cas# 36653-82-4

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols
(Monohydric alcohols) John Wiley & Sons - on line.
03-JAN-2006 (16) (50) (67)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Species	:	other: New Zealand White rabbit
Concentration	:	undiluted
Dose	:	.1 ml
Exposure Time	:	
Comment	:	not rinsed
Number of animals	:	3
Result	:	not irritating
EC classification	:	not irritating
Method	:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	:	1987
GLP	:	yes
Test substance	:	octadecanol (112-92-5)
Test substance	:	Tradename Kalcol 8098
Test condition	:	TEST ANIMALS: Rabbit - Strain: New Zealand White - Sex: 1 male, 2 females - Source: David Percival Ltd, Cheshire, UK - Age: 12-16 weeks - Weight at study initiation: 2.90-3.23 kg - Number of animals: 3 - Controls: Untreated eye used as control ADMINISTRATION/EXPOSURE - Preparation of test substance: the substance was a solid and was applied using an adapted syringe. - Amount of substance instilled: 0.1 ml (ca 82 mg) - Vehicle: None - Postexposure period: 72 hours EXAMINATIONS - Scoring system: Draize and modified Kay and Callandra. - Observation period: 72 hours - Tool used to assess score: Standard ophthalmoscope.
Result	:	AVERAGE SCORE (24+48+72 hour)

- Cornea: 0, 0, 0.3 (group mean score 0.1)
- Iris: 0, 0, 0.3 (group mean score 0.1)
- Conjunctivae (Redness): 0.3, 0, 1 (group mean score 0.43)
- Conjunctivae (Chemosis): 0, 0, 0.3 (group mean score 0.1)
- Overall irritation score: maximum group mean score 10.0 at 1 hour post instillation. Classified as a mild irritant.

DESCRIPTION OF LESIONS: The application of the test material produced diffuse corneal opacity restricted to one treated eye at 24 hours. Iridial inflammation was noted in 2 eyes at 1 hour and one at 24 hours. Minimal to moderate conjunctival irritation was reported at 1 hour with minimal conjunctivitis in 2 eyes at 24 hours.

REVERSIBILITY: All eyes scored 0 at 48 and 72 hours post instillation.

OTHER EFFECTS: Residual test material noted around all eyes at the 1 hour observation period.

Conclusion : Kalcol 8098 is not an eye irritant according to EU or GHS criteria.

Reliability : (1) valid without restriction
Guideline study

Source : Sanders 1996h
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Sanders, A. 1996h. Kalcol 8098: Acute eye irritation test in the rabbit. SPL Project Number 140/504.

04.01.2006 (19)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Test substance: >= 90% 1-eicosanol (629-96-9)

Remark: Summary report of rabbit eye irritation test (OECD 405). The test material was reported as slightly irritating.

Eye irritation study of Nacol 20 in the rabbit. Laboratory of Pharmacology & Toxicology, for Condea Chemie GmbH, 1986

Test substance: Tradename Nacol 20

Reliability: (4) not assignable
Secondary reference. (Study appears to be guideline and conducted at a contract laboratory but there are no supporting details)

Reference: Iuclid 2000 European Commission - European Chemicals Bureau
Icosan-1-ol Cas# 629-96-9.

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Species: rabbit
Concentration: undiluted
Dose: .1 ml
Comment: not rinsed
No. of Animals: 3
Vehicle: none
Result: slightly irritating
EC classificat.: not irritating

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1997
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)
Result: AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): 0.53 (individual 24+48+72 hour mean scores 1, 0.3, 0.3).
- Conjunctivae (Chemosis): 0.1 (individual 24+48+72 hour mean scores 0.3, 0, 0)
- Overall irritation score: maximum group mean score (Draize 10.7).

DESCRIPTION OF LESIONS: Moderate conjunctival irritation was reported in all animals one hour after treatment with minimal to moderate conjunctival irritation at the 24 hour observation time. At 48 hours minimal conjunctival redness was observed in one animal only.

REVERSIBILITY: All scores were 0 at 72 hours.

OTHER EFFECTS: None reported.
Source: Hempstock, 1997e
Hayes Consultancy Service Bromley, Kent
Test condition: TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: 1 female, 2 males
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.80-2.90kg
- Number of animals: 3
- Controls: Untreated eye used as control

ADMINISTRATION/EXPOSURE
- Preparation of test substance: the substance was a solid and was applied using an adapted syringe.
- Amount of substance instilled: 0.1 ml (ca 62 mg)
- Vehicle: None
- Postexposure period: 72 hours

EXAMINATIONS
- Scoring system: Draize and modified Kay and Callandra.
- Observation period: 72 hours
- Tool used to assess score: Standard ophthalmoscope.

Test substance: Tradename Kalcol 220-80
Conclusion: Kalcol is not classifiable as an eye irritant according to EU or GHS criteria.
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
Reference: Hempstock, 1997e Kalcol 220-80: Acute eye irritation test in the rabbit SPL Project Number: 140/722.
06-AUG-2005 (11)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Test substance: >95% 1-docosanol (661-19-8)

Remark: Secondary report of data from Laboratory of Pharmacology and Toxicology, 1986 cited in Iuclid 2000. Eye irritation study of Nacol 22 RD in the rabbit after single instillation into the conjunctival sac.

Study to OECD guideline 405, no further details available. Nacol 22 RD was not irritating to the eye.
Test substance: Tradename Nacol 22RD
Reliability: (4) not assignable
Secondary reference.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau Docosan-1-ol Cas# 661-19-8.
06-AUG-2005 (17)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Remark: Summary report of an unpublished study from Henkel, 1977. 50 ul of a 1% dilution of behenyl alcohol in olive oil was instilled into the conjunctival sac of 5 rabbits. No further details available. Conjunctival irritation was scored at 2, 6, 24 and 48 hours postinstillation according to Draize, 1959. There were no corneal or iritic effects. Conjunctival

irritation was observed at 2 and 6 hours postinstillation with mean conjunctival irritation scores of 18 and 10 respectively. There were no signs of conjunctival irritation at 24 and 48 hours. Based on these scores behenyl alcohol is not irritating to the eye.

Test substance: Behenyl alcohol, 1-docosanol (661-19-8)

Reliability: (4) not assignable
Secondary reference.

Reference: Cosmetic Ingredient Review (CIR) 1988 Final report on the safety assessment of cetearyl alcohol, cetyl alcohol, isostearyl alcohol, myristyl alcohol and behenyl alcohol. J. Am. Coll. Tox. 7(3):359-413

19-OCT-2004 (9)

<u>1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)</u>

Remark: 1-Triacontanol caused severe irritation in rabbits. No further details available.

Reliability: (4) not assignable

Reference: EPA (1983). US Environmental Protection Agency. Tolerances and Exemptions from Tolerances for Pesticide Chemical in or on Raw Agricultural Commodities: 1-Triacontanol. Fed. Reg. 48, (92), 21132.

05-APR-2007

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5.3 Sensitization

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Mouse ear swelling test
Species	Mouse
Number of animals	23
Vehicle	
Result	not sensitizing
Classification	not sensitizing
Method	other
Year	1988
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Age at start of treatment: 6-8 weeks Acclimation: 7 days
Result	On day 0, mice (9 males and 10 females) were injected s.c. with 0.05 ml of the test substance in complete Freund's adjuvant (scapular region) and the test substance was also applied topically to the abdomen (amount not specified). On days 3, 5, 7, 10, 12 and 14 they received topical applications to the shaved abdomen, and a second scapular s.c. injection of 0.05 ml in CFA was given on day 7. On day 26, the thickness of the left ear was measured using a mobile disk caliper with an accuracy of 0.01 mm immediately prior to application of the test substance to both sides of the ear. Left ear thickness was measured again on days 27 and 28 (i.e. 24 and 48 hours after challenge). No increase in ear thickness following challenge application of ethanol. Measurement of 94 untreated mice showed an ear thickness of 0.214 mm with a typical variation of 0.002 mm. There was no statistically significant increase in ear thickness following challenge application of ethanol. Average ear thickness before: 21.66 +- 1.85 mm. Average thickness after: 21.69 +/- 1.91 (Swelling 0.1 %). Known moderate and strong sensitizers applied as controls produced significant swelling in this study.
Test substance	Test substance was 95% ethanol.
Reliability	(2) valid with restrictions
Flag	Critical study for SIDS endpoint
Reference	Descotes, J. (1988). Identification of contact allergens: the mouse ear sensitization assay. J Toxicol-Cut & Ocular Toxicol 7: 263-272.
12.11.2004	(197)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Guinea pig maximization test
Species	guinea pig
Number of animals	10
Vehicle	
Result	not sensitizing
Classification	not sensitizing
Method	other
Year	1984
GLP	yes
Test substance	ethanol (64-17-5)
Remark	Effective concentrations of ethanol used in the induction phase were: Subst. 1; intradermal: 25% Subst. 1; topical: 37.5% Subst. 2 intradermal and topical: 37.5% Effective concentrations of ethanol used in the challenge phase: Subst. 1 1st and 2nd challenges: 25%, 47.5% Subst. 21st Challenge: 37.5%, 60% and 71.25% Subst. 2 2nd Challenge: 22.5%, 60% and 71.25% Method: Test procedure was based on that of Magnusson and Kligman (1969) J. Invest. Derm. ,52,269. Test animals were femnale Dunkin-Hartley albino guinea pigs; 10 test and 10 controls.
Result	No skin reactions were evoked at challenge with the polyalkalene glycol in 75% ethanol in either test or control group animals. Although this study was not primarily carried out to assess ethanol, it can be reliably concluded that ethanol did not show any signs of sensitizing propert
Reliability	(2) valid with restrictions There is no detailed information provided on method used other than reference to a second source document. No positive control was used.
Flag	Critical study for SIDS endpoint
Reference	BP Chemicals Ltd (1984). Results of the Biological Investigations on Selected Materials of the Breox Polyalkylene Glycol Block Copolymer Range. BP Group Occupational Health Centre Toxicology Report 25-90-0150.
12.11.2004	(198)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: other: modified Draize test
Species: other: inbred Hartley albino guinea pigs
Concentration 1st: Induction .25 % intracutaneous
2nd: Challenge 10 % open epicutaneous
3rd: Challenge .1 % intracutaneous
No. of Animals: 10
Vehicle: no data
Result: not sensitizing
Classification: not sensitizing

Method: other
Year: 1978
GLP: no data
Test substance: other TS: hexanol (random sample from commercial batch)

Result: RESULTS OF PILOT STUDY: 0.25%, 0.1% and 10% solutions were chosen for the intradermal induction, intradermal challenge and topical challenge respectively.

RESULTS OF TEST
- Sensitization reaction: No sensitisation reactions at challenge or rechallenge following a second induction procedure. The result was reported as non-sensitising, individual animal data were not presented.
- Clinical signs: None
- Rechallenge: No sensitisation

Source: Sharp 1978
Hayes Consultancy Service Bromley, Kent
Test condition: TEST ANIMAL Guinea pig
- Strain: Hartley
- Sex: not reported
- Source: not reported
- Weight at study initiation: ca 350 g
- Number of animals: 10
- Controls: only at rechallenge

ADMINISTRATION/EXPOSURE
- Study type: Non-adjuvant
- Preparation of test substance for induction: not reported, 0.1 ml of the test solution was administered.
- Induction schedule: 4 intradermal injections at one time point over the 2 auxillary and 2 inguinal lymph nodes.
- Concentrations used for induction: Based on a primary irritation screen the concentration used was 2.5 times the

injection challenge concentration (the concentration giving slight barely perceptible irritation with no oedema).
- Challenge schedule: 14 days after induction each animal received an intradermal injection in one flank and a topical application on the other.
- Concentrations used for challenge: 0.1% intradermally ad 10% topically
- Rechallenge: Where materials test negative at challenge a repeat set of induction applications was carried out followed by challenge at 14 days and rechallenge (with controls) 7 days later.
- Positive control: not reported

EXAMINATIONS
- Grading system: A colour matching lighting unit was used to examine the skin reactions. Each injection reaction was scored based on size, erythema and oedema and considered positive if the total score was greater than the total average of the control scores. Application reactions were scored on a scale of 0 to +++ and considered positive if individual reactions were => + and there was no erythema in the controls.

- Pilot study: A preliminary irritation study was undertaken to determine the injection challenge concentration (the concentration giving slight barely perceptible irritation with no oedema) and the application challenge concentration (the highest concentration producing no irritation).

Conclusion: In this non-adjuvant procedure (modified Draize) hexanol was not a skin sensitiser in guinea pigs following intradermal and

topical challenge after 2 series of induction applications.

Reliability: (2) valid with restrictions
Reasonable reporting of a modified Draize test, result reporting limited. Test sample not fully characterised. Controls only included at rechallenge.

Flag: Critical study for SIDS endpoint

Reference: Sharp, D.W. 1978. The sensitization potential of some perfume ingredients tested using a modified Draize procedure. Toxicology 9(3):261-271.

28-DEC-2005 (64)

<u>1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)</u>

Type: Patch-Test
Species: human

Method: other: human patch test
Year: 1975
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Remark: These secondary references report that in a human patch test 1-hexanol (1% in petrolatum) was not a skin irritant or sensitiser.
Reliability: (4) not assignable
Secondary literature.
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3.

Opdyke, D.L.J. 1975 Fragrance raw material monographs - Alcohol C6. 13 (Suppl.) 695-696.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.
12-SEP-2004 (29) (46) (48)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Remark: Report of an M&K guinea pig maximisation test carried out by Henkel (report TBD 790129 also reported in Henkel report TBD900320). The test substance as prescribed was not a skin sensitiser.
Test substance: 1-hexanol
Reliability: (4) not assignable
Secondary reference
Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3.
13-OCT-2004 (29)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: other:maximisation test
Species: other: man
No. of Animals: 25
Vehicle: petrolatum
Result: not sensitizing
Classification: not sensitizing

Method: other: Kligman human maximization test
Year: 1973
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Remark: This reference gives a summary report of unpublished data provided by Kligman 1972.

Also cited in Iuclid 2000 and Patty 2001.

Result: Under the conditions of this test 1-octanol was not a human skin sensitiser.

Source: Opdyke, 1973.
Hayes Consultancy Service Bromley, Kent

Test condition: This patch test was carried out using the maximization procedure described by Kligman, A.M.the identification of contact allergens by human assay. III The maximization test: A procedure for screening and rating contact allergens. J. Invest. Dermatol. 47:393-409, 1966. There are variations in this procedure but we have no information as to which variation was used. The exposure would have been a 48 hour occlusive exposure and sodium lauryl sulphate may have been used to promote the response. The only experimental detail given for 1-octanol was that a panel of 25 volunteers were tested at a concentration of 2% in petrolatum. there is no indication as to whether this was an induction or challenge concentration.

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Octan-1-ol Cas# 111-87-5.

Opdyke, D.L.J. 1973 Monographs on fragrance raw materials. Fd. Cos. Tox. 11: 95-115.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

11-NOV-2004 (62) (88) (90)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Type: other: modified Draize test
Species: other: inbred Hartley albino guinea pigs
Concentration 1st: Induction 1.9 % intracutaneous
2nd: Challenge 10 % open epicutaneous
3rd: Challenge .75 % intracutaneous
No. of Animals: 10
Vehicle: no data

Method: other: modified Draize test
Year: 1978

GLP: no data
Test substance: other TS: decanol (random sample from commercial batch)

Result: RESULTS OF PILOT STUDY: 1.9%, 0.75% and 10% solutions were chosen for the intradermal induction, intradermal challenge and topical challenge respectively.

RESULTS OF TEST
- Sensitization reaction: No sensitisation following the original induction procedure. Individual animal data not reported. Sensitisation is reported after a second induction series however the actual number of animals responding is not reported. This suggests that the sample of decanol tested is at most a weak sensitiser. The authors note that they frequently find that weak sensitisers identifed by this repeated induction procedure do not induce sensitization in their guinea pig test when tested as an ingredient of perfume formulations. They also state that decanol did not produce sensitisation in the human maximisation test.
- Clinical signs: None
- Rechallenge: Sensitisation observed on challenge and/or rechallenge following a second induction procedure.

Source: Sharp, 1978
Test condition: TEST ANIMAL Guinea pig
- Strain: Hartley
- Sex: not reported
- Source: not reported
- Weight at study initiation: ca 350 g
- Number of animals: 10
- Controls: only at rechallenge

ADMINISTRATION/EXPOSURE
- Study type: Non-adjuvant
- Preparation of test substance for induction: not reported, 0.1 ml of the test solution was administered.
- Induction schedule: 4 intradermal injections at one time point over the 2 auxillary and 2 inguinal lymph nodes.
- Concentrations used for induction: Based on a primary irritation screen the concentration used was 2.5 times the injection challenge concentration (the concentration giving slight barely perceptible irritation with no oedema).
- Challenge schedule: 14 days after induction each animal received an intradermal injection in one flank and a topical application on the other.
- Concentrations used for challenge: 0.1% intradermally and 10% topically

- Rechallenge: yes 7 days later if positive. If negative the induction procedure was repeated with subsequent challenge and rechallenge as appropriate, this time with controls at rechallenge.
- Positive control: not reported

EXAMINATIONS
- Grading system: A colour matching lighting unit was used to examine the skin reactions. Each injection reaction was scored based on size, erythema and oedema and considered positive if the total score was greater than the total average of the control scores. Application reactions were scored on a scale of 0 to +++ and considered positive if individual reactions were => + and there was no erythema in the controls.
- Pilot study: A preliminary irritation study was undertaken to determine the injection challenge concentration (the concentration giving slight barely perceptible irritation with no oedema) and the application challenge concentration (the highest concentration producing no irritation).

Conclusion: In this non-adjuvant procedure (modified Draize) decanol produced a weak sensitisation reaction in guinea pigs only after two sets of induction injections and following topical and/or intradermal challenge. The authors note that they frequently find that weak sensitisers identifed by this procedure do not induce sensitization in their guinea pig test when tested as an ingredient of perfume formulations. They also state that decanol did not produce sensitisation in the human maximisation test.

Reliability: (2) valid with restrictions
Reasonable reporting of a modified Draize test, result reporting limited. Test sample not characterised.

Flag: Critical study for SIDS endpoint

Reference: Sharp, D.W. 1978. The sensitization potential of some perfume ingredients tested using a modified Draize procedure. Toxicology 9(3): 261-271.

30-DEC-2005 (82)

<u>1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)</u>

Type: other: human maximization test
Species: human
No. of Animals: 25
Vehicle: petrolatum
Result: not sensitizing
Classification: not sensitizing

Method: other: Kligman human maximization test
Year: 1973
GLP: no
Test substance: > 90% 1-decanol (112-30-1)

Remark: This reference reports in summary unpublished data provided by Kligman 1972.
Result: Under the conditions of this test 1-decanol was not a human skin sensitiser.
Source: Opdyke, 1973
Hayes Consultancy Service Bromley, Kent
Test condition: This patch test was carried out using the maximization procedure described by Kligman, A.M. The identification of contact allergens by human assay. III The maximization test: A procedure for screening and rating contact allergens. J. Invest. Dermatol. 47:393-409, 1966. There are variations in this procedure but we have no information as to which variation was used. The exposure would have been a 48 hour occlusive exposure and sodium lauryl sulphate may have been used to promote the response. The only experimental detail given for 1-decanol was that a panel of 25 volunteers were tested at a concentration of 2% in petrolatum.
Reliability: (4) not assignable
Documentation insufficient for assessment.
Reference: Iuclid 2000 ECB Decanol.

Opdyke, D.L.J. 1973 Monographs on fragrance raw materials.
Fd. Cos. Tox. 11: 95-115.
25-NOV-2004 (53) (69)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)</u>

Type	:	Guinea pig maximization test
Species	:	other: Hartley albino guinea pigs
Concentration	:	Induction 3 % intracutaneous Induction 50 % occlusive epicutaneous Challenge 10 % occlusive epicutaneous
Number of animals	:	10
Vehicle	:	other: liquid paraffin
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	OECD Guide-line 406 "Skin Sensitization"
Year	:	1997
GLP	:	yes
Test substance	:	dodecanol (112-53-8)

Test substance : Tradename Kalcol 2098

Test condition : TEST ANIMALS: Guinea pigs
- Strain: albino Hartley
- Sex: female
- Source: Japan SLC, Shizuoka
- Age: 4 weeks
- Weight at study initiation: 276-323 g
- Number of animals: 10F
- Controls: 5F

ADMINISTRATION/EXPOSURE
- Study type: adjuvant, maximization test
- Preparation of test substance for induction: In liquid paraffin
- Preparation of test substance for induction: In liquid paraffin
- Induction schedule: Single intradermal injection followed 7 days later by a 48 hour occlusive patch applied topically.
- Concentrations used for induction: 3% intracutaneous, 50% topical
- Concentration in Freuds Complete Adjuvant (FCA): 1:1 water in oil emulsion of 6% test substance in FCA and saline.
- Challenge schedule: 21 days after first induction topical application of an occluded patch for 24 hours.
- Concentrations used for challenge: 3 and 10%
- Rechallenge: No
- Positive control: DNCB and formalin, not concurrent evidence presented over a relevant time period that the strain of guinea pig did respond to known sensitisers.

EXAMINATIONS
- Grading system: 0 = no visible change, 1 = discrete or patch erythema; 2 = moderate and confluent erythema; 3 = intense erythema and swelling.
- Pilot study: Using 4 animals and multiple patches Kalcol 2978 was tested at concentrations from 0.1% - 10% intradermally and at 10, 30 and 100% topically.

Result : RESULTS OF PILOT STUDY: Following intradermal injection significant skin irritation was seen at concentrations of 5 and 10% persisting for 72 hours. The 3% concentration showed evidence of irritation at 24 hours only. Following topical application the undiluted material was irritant up to 48 hours, 2/4 guineapigs showed irritation at 10% while there was no evidence of irritation with the 3% concentration.

RESULTS OF TEST
- Sensitization reaction: There was no evidence of sensitisation in any

of the test animals. Reactions at 24 and 48 hours following challenge with the solvent control (liquid paraffin) and 3% and 10% solutions were 0/10 treated, 0/5 control.
- Clinical signs: There were no significant differences in general condition and body weight gain between test and control groups over the course of the test.
- Rechallenge: Not required.

Conclusion : Kalcol 2078 is not a skin sensitiser when tested according to the M&K maximisation procedure.

Reliability : (1) valid without restriction
Guideline study

Source : Iihama 1997a
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference
07.12.2005

Iihama, K. 1997a. The maximization test for contact hypersensitivity potential of Kalcol 2098 in guinea pigs. Test Number 9718. (15)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Type: Guinea pig maximization test
Species: other: Hartley albino guinea pigs
Concentration 1st: Induction 5 % intracutaneous
2nd: Induction 50 % occlusive epicutaneous
3rd: Challenge occlusive epicutaneous
No. of Animals: 10
Vehicle: other: liquid paraffin
Result: not sensitizing
Classification: not sensitizing

Method: OECD Guide-line 406 "Skin Sensitization"
Year: 1997
GLP: yes
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: RESULTS OF PILOT STUDY: Following intradermal injection skin irritation was seen at concentrations of 10% and 5% persisting for 72 hours but less marked at the lower concentration. The 3% concentration showed evidence of irritation at 24 hours in one animal only. Loweer concentrations from 0.1 -1% showed no irritation. Following topical application slight irritation was seen in 2/4 animals at 50% only.

RESULTS OF TEST
- Sensitization reaction: There was no evidence of sensitisation in any of the test or control animals at either challenge concentration. Response 0/10 test, 0/5 control.
- Clinical signs: There were no significant differences in general condition and body weight gain between test and control groups over the course of the test.
- Rechallenge: Not required.

Source: Iihama 1997b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ANIMALS: Guinea pigs
- Strain: albino Hartley
- Sex: female
- Source: Japan SLC, Shizuoka
- Age: 4 weeks
- Weight at study initiation: 276-323 g
- Number of animals: 10F
- Controls: 5F

ADMINISTRATION/EXPOSURE
- Study type: adjuvant, maximization test
- Preparation of test substance for induction: In liquid paraffin
- Preparation of test substance for induction: In liquid paraffin
- Induction schedule: Single intradermal injection followed 7 days later by a 48 hour occlusive patch applied topically.
- Concentrations used for induction: 5% intracutaneous, 50% topical
- Concentration in Freuds Complete Adjuvant (FCA): 1:1 water in oil emulsion of 10% test substance in FCA and saline.
- Challenge schedule: 21 days after first induction topical application of an occluded patch for 24 hours.
- Concentrations used for challenge: 3 and 10%
- Rechallenge: No
- Positive control: DNCB and formalin, not concurrent, evidence presented over a relevant time period that the strain of guinea pig did respond to known sensitisers.

EXAMINATIONS
- Grading system: 0 = no visible change, 1 = discrete or patch erythema; 2 = moderate and confluent erythema; 3 = intense erythema and swelling.
- Pilot study: Using 4 animals and multiple patches Kalcol

4098 was tested at concentrations from 0.1% - 10% intradermally and at 3, 10, and 50% topically.
Test substance: Tradename Kalcol 4098.
Conclusion: Kalcol 4098 is not a skin sensitiser when tested according to the M&K maximisation procedure.
Reliability: (1) valid without restriction
Guideline study.
Flag: Critical study for SIDS endpoint
Reference: Iihama, K. 1997b. The maximization test for contact hypersensitivity potential of Kalcol 4098 in guinea pigs. Test Number 9719.
05-DEC-2005 (42)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Type: other: human maximisation test
Species: human
No. of Animals: 50
Vehicle: petrolatum
Result: not sensitizing

Method: other: human maximisation test
Year: 1974
GLP: no data
Test substance: > 95% 1-Tetradecanol (112-72-1)

Remark: Tetradecanol at a concentration of 12% in petrolatum was tested in two series of 25 human volunteers using the numan maximisation procedure of Kligman 1966 and Kligman & Epstein, 1975. In the first panel sensitisation reactions were reported in 2/25 volunteers. No sensitisation reactions were observed in the second test panel. Overall it appears that tetradecanol is not a skin senisiter in man.

Secondary reference report of unpublished data from Kligman 1974.
Source: Hayes Consultancy Service Bromley, Kent
Reliability: (4) not assignable
Secondary reference.
Reference: Opdyke, D.L.J. 1975 Fragrance raw material monographs - Alcohol C14 Myristic. 13 (Suppl.) 699-700.
16-JUL-2005 (53)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: Guinea pig maximization test

Species: other: albino Dunkin Hartley guinea pig
Concentration 1st: Induction 1 % intracutaneous
2nd: Induction 50 % occlusive epicutaneous
3rd: Challenge occlusive epicutaneous
No. of Animals: 15
Vehicle: other: arachis oil
Result: not sensitizing
Classification: not sensitizing

Method: OECD Guide-line 406 "Skin Sensitization"
Year: 1996
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: RESULTS OF PILOT STUDY: Intradermal. Erythema (grade 2) observed at all injection sites, no systemic toxicity. Tested at 1% only. Topical application for induction (48 hour) minimal irritation at 5 and 10%, with 25 and 50% maximum erythema score 2 persisting to 48 hours after removal of patch. Topical application for challenge initial minimal response at 1 hour, no irritation at 24 and 48 hours.

RESULTS OF TEST
- Sensitization reaction: No sensitisation reaction in any of the test or control animals. Response 0/10 test, 0/5 controls.
- Clinical signs: Body weights and weight gain over the observation period were comparable in test and control groups. One animal was killed after topical challenge, the reason was not given but this was not considered to affect the results of the test. Well defined - moderate erythema at the intradermal injection site 24 hours after induction, well defined erythema at 48 hours. Following topical induction very slight to well defined erythema was noted 1 hour after patch removal, very slight erythema observed in 2/10 test animals at 24 hours. No skin reactions following topical challenge.
- Rechallenge: Not required.

Source: Driscoll 1996a
Hayes Consultancy Service Bromley, Kent
Test condition: TEST ANIMALS: Guinea pigs
- Strain: Dunkin Hartley
- Sex: male
- Source: David Hall, Staffs, UK
- Age: 8-12 weeks
- Weight at study initiation: 376 -454 g
- Number of animals: 10
- Controls: 5

ADMINISTRATION/EXPOSURE
- Study type: M&K maximisation procedure (adjuvant method)
- Preparation of test substance for induction: in arachis oil
- Induction schedule: Day 1 intradermal induction, day 7 topical induction (48 hours occlusive).
- Concentrations used for induction: intradermal 1% in arachis oil, topical 50% in arachis oil.
- Concentration in Freuds Complete Adjuvant (FCA): 1%
- Challenge schedule: Day 21 topical challenge (24 hours occlusive)
- Concentrations used for challenge: 25 and 50% in arachis oil.
- Rechallenge: No
- Positive control: Evidence of reaction of the strain of guinea pigs to known skin sensitisers over an appropriate period was provided.

EXAMINATIONS
- Grading system: Draize 0-4 scale for erythema and oedema.
- Pilot study: Topical (24 and 48 hour occlusive) applications were tested at 5, 10, 25 and 50%. Intradermal injection was carried out at 1% the maximum suitable concentration.

Test substance: Tradename Kalcol 6098
Conclusion: Kalcol 6098 is not a skin sensitiser in the guinea pig when tested using the Magnusson and Kligman maximisation assay.
Reliability: (1) valid without restriction
Guideline study.
Flag: Critical study for SIDS endpoint
Reference: Driscoll, R. 1996a. Kalcohl 6098: Magnusson & Kilgman maximization study in the guinea pigs. SPL Project Number 140/497.
05-DEC-2005 (21)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Type: Guinea pig maximization test
Species: guinea pig
Concentration 1st: Induction 5 % intracutaneous
2nd: Induction 5 % occlusive epicutaneous
3rd: Challenge 25 % open epicutaneous
No. of Animals: 20
Vehicle: other: olive oil, vaseline or ethanol
Result: not sensitizing
Classification: not sensitizing

Method: other: Magnusson & Kligman, 1969
Year: 1983
GLP: no data
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: RESULTS OF TEST
- Sensitization reaction: Response 0/20 test, 0/20 control
- Clinical signs: None
- Rechallenge: Not required

Test condition: TEST ANIMALS: Guinea pigs
- Strain: Pirbright white
- Sex: no data
- Source: no data
- Weight at study initiation: 400 - 500g
- Number of animals: 20
- Controls: 20

ADMINISTRATION/EXPOSURE
- Study type: adjuvant
- Preparation of test substance for intradermal induction: 5% in olive oil
- Preparation of test substance for topical induction: 5% in vaseline
- Induction schedule: 6 intracutaneous injections and patch tests. As described by Magnusson & Kligman, 1969.
- Concentration in Freuds Complete Adjuvant (FCA): 1:1
- Challenge schedule: As described by Magnusson & Kligman, 1969
- Concentrations used for challenge: 25% in vaseline or ethanol.
- Rechallenge: no
- Positive control: Not reported.

Conclusion: 1-hexadecanol is not a skin sensitiser when tested using the M&K maximisation procedure. Results cited in Iuclid 2000.
Reliability: (2) valid with restrictions
Publication, reasonable documentation, meets generally accepted scientific principles, acceptable for assessment.
Flag: Critical study for SIDS endpoint
Reference: Gloxhuber, Ch. (1983) Berwertung der allergologischen Eigenschaften von Cetyl- und Stearylalkohol. Aerztliche Kosmetologies 13:181-186.

Iuclid 2000 European Commission - European Chemicals Bureau
Hexadecan-1-ol Cas# 36653-82-4
05-DEC-2005 (33) (50)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Remark: Secondary report of unpublished data. A maximisation test was carried out on 26 human volunteers with hexadecanol at a concentration of 12% in petrolatum. There were no sensitisation reactions.

The same Iuclid 2000 record reports a case of urticaria-like dermatitis in a 28 year old white female. No further details available.

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Reliability: (4) not assignable
Secondary reference.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Hexadecan-1-ol Cas# 36653-82-4.

Opdyke, D.L.J. 1978 Fragrance raw materials monographs Fd. Cos. Tox. 16: 683-686.

Patty, F.A (ed) 1963 Industrial Hygiene and Toxicology 2nd revised edition Vol. 11 Toxicology Chapter 34 Alcohols (J.F. Treon) Interscience publishers.

05-DEC-2005 (50) (66) (68)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Type	:	Guinea pig maximization test
Species	:	other: albino Dunkin Hartley guinea pig
Concentration	:	Induction 1 % intracutaneous Induction 50 % occlusive epicutaneous Challenge occlusive epicutaneous
Number of animals	:	10
Vehicle	:	other: arachis oil
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	OECD Guide-line 406 "Skin Sensitization"
Year	:	1996
GLP	:	yes
Test substance	:	octadecanol (112-92-5)
Test substance	:	Tradename Kalcol 8098
Test condition	:	TEST ANIMALS: Guinea pigs - Strain: Dunkin Hartley - Sex: male - Source: David Hall, Staffs, UK

- Age: 8-12 weeks
- Weight at study initiation: 305 -419 g
- Number of animals: 10
- Controls: 5

ADMINISTRATION/EXPOSURE
- Study type: M&K maximisation procedure (adjuvant method)
- Preparation of test substance for induction: in arachis oil
- Induction schedule: Day 1 intradermal induction, day 7 topical induction (48 hours occlusive).
- Concentrations used for induction: intradermal 1% in arachis oil, topical 50% in arachis oil.
- Concentration in Freuds Complete Adjuvant (FCA): 1%
- Challenge schedule: Day 21 topical challenge (24 hours occlusive)
- Concentrations used for challenge: 25 and 50% in arachis oil.
- Rechallenge: No
- Positive control: Evidence of reaction of the strain of guinea pigs to known skin sensitisers over an appropriate period was provided.

EXAMINATIONS
- Grading system: Draize 0-4 scale for erythema and oedema.
- Pilot study: Topical (24 and 48 hour occlusive) applications were tested at 5, 10, 25 and 50%. Intradermal injection was attempted at 1 and 5% but the 5% solution was impossible to inject.

Result : RESULTS OF PILOT STUDY: Minimal erythema at 24 and 48 hours after 48 hour topical exposure, no irritation at these time periods after a 24 hour topical application. Well defined erythema (grade 2) at 24, 48 and 72 hours post injection reducing to slight erythema (grade 1) at 7 days.

RESULTS OF TEST
- Sensitization reaction: No positive responses with 25% or 50% challenge concentrations in test or control groups at 24 or 48 hours. 0/10 treated and 0/5 controls responded to challenge.
- Clinical signs: Body weights and weight gain over the observation period were comparable in test and control groups. Well-defined erythema was noted at the intradermal induction sites of all test group animals at 24 and 48hours. Very slight to well-defined erythema was noted at the intradermal sites of the control group at 24 and very slight erythema at 3 sites at 48 hours.
Very slight to well-defined erythema was noted at the induction sites of six test group animals at the 1 hour mark. No skin reactions were noted at the induction sites of any test group animals at the 24 hour mark.
- Rechallenge: Not carried out.

Conclusion	:	Kalcol 8098 is not a skin sensitiser when tested using the Magnusson and Kligman guinea pig maximization procedure.
Reliability	:	(1) valid without restriction Guideline study
Source	:	Driscoll 1996b Hayes Consultancy Service Bromley, Kent
Flag	:	Critical study for SIDS endpoint
Reference		Driscoll, R. 1996b. Kalcohl 8098: Magnusson & Kilgman maximization study in the guinea pigs. SPL Project Number 140/503.
07.12.2005		(6)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Remark: Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18, all assays were negative. Included are negative data from guinea pig maximisation tests for C16 (hexadecanol) and C18 (octadecanol) which support the conclusion that C20 alcohols are not expected to be skin sensitisers.
Test substance: >= 90% 1-eicosanol (629-96-9)
Conclusion: Not expected to be a skin sensitiser.
Reliability: (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
Reference: SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category
15-SEP-2005 (18) (23)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Remark: Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18, all assays were negative. Included are negative data from guinea pig maximisation tests for, C16 (hexadecanol), C18 (octadecanol) which support the conclusion that C22 alcohols are not expected to be a skin sensitisers.
Test substance: >95% 1-docosanol (661-19-8)
Conclusion: Not expected to be a skin sensitiser.

Reliability: (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category
15-SEP-2005 (26) (29)

5.4 Repeated Dose Toxicity

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Sub-chronic
Species	Rat
Sex	male/female
Strain	Sprague-Dawley
Route of admin.	oral feed
Exposure period	90 days
Frequency of treatm.	Daily
Post exposure period	
Doses	1, 2, 3, 4, 5%,10% w/w ethanol in liquid diet
Control group	
NOAEL	= 2%
LOAEL	= 3%
Method	other
Year	1986
GLP	no data
Test substance	other TS: pure ethanol (64-17-5)

Method

Age at study start: 43 days No. of animals per sexper dose: 10
Ethanol supplied in nutritionally balanced liquid diet.
Controls received diet without ethanol.
Parameters recorded: Bodywelghts weekly, food consumption daily.
Blood aspartate aminotransferase and alanine aminotransferase levels determined at termination.
Liver and kidneys were examined macroscopically and microscopically at necropsy and the spleen was weighed.

	No statistical tests for significance were used.
Remark	2% dose calculated to be equivalent to 2400mg/kg/day
Result	Bodyweight: All groups gained weight though final weights decreased with dose. Food/water consumption: Consumption in the 10% group was reduced relative to controls (182 ml diet/kg-d versus 195 ml diet/kg-d). Clinical signs: No adverse signs were observed Ophthalmology, haematology: Not examined. Clinical biochemistry: Serum liver enzymes were not affected by treatment and kidney findings were minimal. Mortality and time to death: No deaths occurred. Fross pathology: Liver yellowing, dosage~related. Histopathology: Hepatic centrilobular steatosis increased in severity with dose as did the frequency and severity of Mallory bodies (hyaline) and acidophilic degeneration and necrosis. Most liver findings were absent or mild at 2% w/w ethanol but became more significant at 3% and higher dose. Reticulo-endothelial cell proliferation was slight at t and 2%. A few kidney casts were noted in animals from the 1-3% dose groups and there were a few calcifications in the 3-5% groups. Slight tubular fatty change occurred in all groups.
Reliability	(2) valid with restrictions
Flag	Critical study for SIDS endpoint
Reference	Holmberg, S., Kronevi, T., Ekner, A. (1986). Subchronic toxicity investigation of ethyl alcohol: a test for lowest effective dose (led) to be used in a long term bioassay for carcinogenicity. National Board of Occupational Safety and Health, Solna, Sweden.
12.11.2004	(199)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-chronic
Species	Mouse
Sex	Male
Strain	B6C3F1
Route of admin.	drinking water
Exposure period	90 days
Frequency of treatm.	7 days/week ad libitum
Post exposure period	
Doses	5% w/v in deionized water
Control group	yes, concurrent vehicle
NOAEL	< 5%
LOAEL	= 5%
Method	other: NTP 13-wk toxicity protocol

Year	1996
GLP	Yes
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Age at study start: 43-46 days Number of animals per sex per group: 10 Ethanol was diluted in deionized water. No satellite animals were included. Parameters observed were bodyweights, water consumption and clinical observations weekly. Sperm motility was assessed at termination. Complete necropsies were performed. Statistical tests were t-tests and F-tests.
Remark	The 5% dose was calculated as equivalent to 7300-9400 mg/kg body weight over the various urethane dose groups, based on average body weight and drinking water consumption.
Result	LOAEL dose was much greater than 5% wlv for observed body and organ weight increases and decreased sperm count. No premature deaths occurred. Bodyweight-relative liver weight was increased and there were increases in absolute heart, liver, kidney and lung weight Minimal nephropathy occurred in 30% of treated animals and in 10% controls. Sperm count in the cauda epididymis was decreased.
Source	U.S. Environment Protection Agency High Production Volume, Chemical Right to Know Program.
Reliability	(2) valid with restrictions Single dose used did not allow a NOAEL to be determined so therefore only reliable with restrictions.
Reference	National Toxicology Program (1996). NTP Technical Report on Toxicity Studies on Urethane in Drinking water and Urethane in 5% Ethanol Administered to F344 Rats and B6C3F1 Mice. NTP, Research Triangle Park, NC, USA.
12.11.2004	(200)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-chronic
Species	Mouse
Sex	Female
Strain	B6C3F1
Route of admin.	drinking water
Exposure period	90 days

Frequency of treatm.	7 days/week ad libitum
Post exposure period	
Doses	5% w/v in deionized water
Control group	yes, concurrent vehicle
NOAEL	= 5%
LOAEL	> 5%
Method	other: NTP 13-wk toxicity protocol
Year	1996
GLP	Yes
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Age at study start: 43-46 days Number of animals per sex per group: 10 Ethanol was diluted in deionized water. Satellite animals were not included. Parameters observed were bodyweights, water consumption and clinical observations weekly. Vaginal cytology was assessed before termination. Complete necropsies were performed. Statistical tests were t-tests and F-tests. Oestrus cycle length was determined.
Remark	Bodyweight: Unaffected by treatment Food/water consumption: water consumption lowered in ethanol group. Clinical signs: None noted Ophthalmological, haematological and blood chemistry findings: Not examined. Mortality and time of death: No premature deaths occurred. Gross pathology: Time spent in dioestrus and pro-oestrus was increased. Organ weight changes: Ethanol treatment did not affect organ weights. Histopathology: Non-neoplastic lesions did not significantly differ from controls The 5% dose was calculated as equivalent to 17000-24000 mg/kg body weight over the various urethane dose groups, based on average body weight and drinking water consumption.
Result	NOAEL effects were body and organ weights and oestrous cycle length. The only treatment-related change in female mice was the time spent in dioestrus and pro-oestrus but it was unclear whether this was significant. Cycle length was unchanged.
Reliability	(1) valid without restriction Highly reliable. Single dose but sufficient to determine a NOAEL.
Reference	National Toxicology Program (1996). NTP Technical Report on Toxicity Studies on Urethane in Drinking water and Urethane in

	5% Ethanol Administered to F344 Rats and B6C3Ft Mice. NTP, Research Triangle Park, NC, USA
12.11.2004	(201)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Sub-chronic
Species	Rat
Sex	Female
Strain	
Route of admin.	drinking water
Exposure period	90 days
Frequency of treatm.	7 days/week ad libitum
Post exposure period	
Doses	5% w/v in deionized water
Control group	yes, concurrent vehicle
NOAEL	< 5%
LOAEL	= 5%
Method	other: NTP 13-wk toxicity protocol
Year	1996
GLP	Yes
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Age at study start: 43-46 days Number of animals per sex per group: 10 Ethanol was diluted in deionized water. Satellite animals were included for haematological and clinical chemistry examination at 3 and 23 days. Parameters observed were bodyweights, water consumption and clinical observatons weekly. Haematology, blood chemistry and vaginal cytology was assessed before study termination. Complete necropsies were performed. Statistical tests were t-tests and F-tests.
Remark	The 5% dose was calculated as equivalent to 4800-5600 mg/kg body weight over the various urethane dose groups, based on average body weight and drinking water consumption.
Result	Body and organ weights were unaffected by treatment while alanine aminotransferase was decreased and serum bile acids were increased at week 13. NOAEL and LOAEL were not achieved at this dosage. No clinical signs, ophthalmological, haematological, or organ weight changes were observed. No premature deaths occurred. Minimal nephropathy occurred in 40% test animals and in 0% of controls. No liver lesions were found in controls but

	hepatodiaphragmatic nodules were observed in ethanol-exposed animals. (2) valid with restrictions
Reliability	Single dose used did not allow a NOAEL to be determined so therefore only reliable with restrictions.
Reference	National Toxicology Program (1996). NTP Technical Report on Toxicity Studies on Urethane in Drinking water and Urethane in 5% Ethanol Administered to F344 Rats and B6C3F1 Mice. NTP, Research Triangle Park, NC, USA
12.11.2004	(200)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-chronic
Species	Rat
Sex	Male
Strain	Fischer 344
Route of admin.	drinking water
Exposure period	90 days
Frequency of treatm.	7 days/week ad libitum
Post exposure period	
Doses	5% w/v in deionized water
Control group	yes, concurrent vehicle
NOAEL	> 5%
LOAEL	
Method	other: NTP 13-week toxicity protocol
Year	1996
GLP	Yes
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Age at study start: 4346 days Number of animals per sex per group: 10 Ethanol was diluted in deionized water. Satellite animals were included for haematological and clinical chemistry examination at 3 and 23 days. Parameters observed were bodyweights, water consumption and clinical observations weekly. Haematology, blood chemistry and sperm motility was assessed at termination. Complete necropsies were performed. Statistical tests were t-tests and F-tests.
Remark	The 5% dose was calculated as equivalent to 2800-4100 mg/kg body weight over the various urethane dose groups, based on average body weight and drinking water consumption.
Result	There was a 20% decrease in thymus weight relative to controls. Reticulocyte count was increased and serum bile acid

	concentration increased. Some other blood biochemical parameters differed inconsistently from control values at day 3 or 23. Reproductive tissues and sperm counts were not affected by treatment.
Reliability	(1) valid without restriction. Highly reliable. Single dose but sufficient to determine a NOAEL.
Reference	National Toxicology Program (1996). NTP Technical Report on Toxicity Studies on Urethane in Drinking water and Urethane in 5% Ethanol Administered to F344 Rats and B6C3Ft Mice. NTP, Research Triangle Park, NC, USA
12.11.2004	(201)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-chronic
Species	Rat
Sex	no data
Strain	no data
Route of admin.	oral feed
Exposure period	Up to 36 weeks
Frequency of treatm.	Continuous
Post exposure period	None
Doses	2 ml ethanol/rat/day given to 6 rats
Control group	yes, concurrent no treatment
NOAEL	
LOAEL	
Method	other
Year	
GLP	No
Test substance	ethanol (64-17-5)
Remark	Body weight gain decreased in treated rats. Haematological effects evident at all time points ($p < 0.05$) included reductions in erythrocytes, haematocrit and haemoglobin concentration, while erythrocyte sedimentation rate, MCV and MCH were increased. A significant fall in total white bloodcells was also seen in treated rats ($p < 0.001$) at all time points. Lymphocytes were reduced while neutrophils were increased. Monocytes were increased at 10 and 14 weeks only. Six rats given alcohol equivalent to approximately 8 g/kg body weight/day (based on body weight mid-way through the study). Six control rats given isocaloric amount of sucrose. Body weights monitored. Haematological parameters measured after 10, 14, 18 and 22 weeks.
Reliability	(4) not assignable
Reference	Kanwar, K.C. & Tikoo, A. (1992) Hematological lesions in rat

	following heavy alcohol ingestion. J. Env. Path. Toxicol. Oncol. 11, 241-245.
12.11.2004	(202)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Sub-chronic
Species	Rat
Sex	Male
Strain	Wistar
Route of admin.	drinking water
Exposure period	8 month
Frequency of treatm.	Continuous
Post exposure period	None
Doses	ca. 7.7 g/kg body weight/day given to 6 rats.
Control group	Yes
NOAEL	
LOAEL	
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Ethanol was given as a 10% solution in drinking water for 8 months after which a range of haematological parameters was studied. Control rats received pure drinking water.
Result	Body weight gain was unaffected in the treated rats. Following ethanol exposure the osmotic fragility of the erythrocytes was increased. There were no statistically significant effects on haematocrit, haemoglobin concentration, erythrocyte count, reticulocyte count, MCV, MCH or MCHC.
Reliability	(4) not assignable
Reference	Rosin, J. at al. (1988) Studies on the effect of ethanol and/or toluene on rat erythrocytes. J. Appl. Toxicol. 8, 369- 372.
12.11.2004	(204)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Chronic
Species	Other
Sex	male/female
Strain	Other
Route of admin.	Other
Exposure period	up to 5 years
Frequency of treatm.	Continuous
Post exposure period	None

Doses	Ethanol added to diet and drinking water of a group of 4 baboons in increments to reach 25 g/kg body weigh/day after 1 year.
Control group	yes
NOAEL	
LOAEL	
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Ethanol was administered in a semi-liquid diet and also in the drinking water to a treated group of 3 male and 1 femaleanimal and a control group of 1 male and 1 female animals. The baboons were weighed and given blood tests regularly. Liver biopsies were performed every 3 months for 2 years, then every 6 months. The treated baboons were studied for 9, 18, 48 and 60 months. Species: Baboon Strain: Papio
Result	The ethanol-containing diet had no effect on body weight gain. Moderate fatly change was seen in the livers of the animals treated for 18 and 48 months, while the livers of those treated for 9 and 60 months were normal. No cirrhosis was evident at post-mortem. Test substance was absolute alcohol.
Reliability	(4) not assignable
Reference	Ainley, C.C. et al. (1988) Is alcohol hepatotoxic in the baboon? J. Hepatol. 7, 85 - 92.
12.11.2004	(205)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Chronic
Species	Other
Sex	no data
Strain	Other
Route of admin.	oral feed
Exposure period	up to 22 months
Frequency of treatm.	Continuous
Post exposure period	None
Doses	Ethanol added to diet of a group of 9 baboons to provide 50% of their total calorific intake as alcohol.
Control group	Yes
NOAEL	
LOAEL	
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)

Remark	A figure of 80 mg/kg body weight day is given in the paper, which may relate to the total volume of liquid diet consumedor to the mean intake of ethanol (which would equate with 63g ethanol/kg body weight/day). An additional group of 6 treated baboons and their pair-fed controls had been given a solid diet with either ethanol or carbohydrates in the drinking water for periods of from 17 to 34 months. They were then changed to the liquid diet foran average of 17 months. When the ethanol was given in a solid diet, no lesions more severe than fatty liver were seen, while with the liquid diet, one baboon developed hepatitis (after 29 months on the solid and 19 months on theliquid diet), two developed incomplete cirrhosis (after 30 months on the solid and 15 months on the liquid diet) and one developed complete cirrhosis (after 34 months on the solid and 19 months on the liquid diet). Ethanol was administered in a liquid diet to 9 treated baboons and 9 pair-fed controls which were given isocaloric carbohydrate. Liver biopsies were performed at regular intervals. The baboons were exposed for from 8 to 22 months,the average exposure being 15 months. Species: Baboon Strain: Papio hamadryas or olive and yellow
Result	The ethanol-containing diet reduced body weight gain, and inebriation was observed. Fatty liver developed in all treated baboons, and the liver triglyceride content increased progressively. Mild inflammation, cellular degeneration and and some fibrosis were noted in the liver, and ultrastructural changes were seen In the mitochondria and endoplasmic reticulum. Three baboons fed ethanol for 9 months, and one treated for 12 months developed alcoholic hepatitis. When two of these animals were biopsied at 20 months, cirrhosis was found. Serum cholesterol and gutamic-oxaloacetic transaminase activity were increased in the treated animals, while haematocrit and haemoglobin values tended to be lower.
Reliability	(4) not assignable
Reference	Lieber, e.s. et al. (1975) Silquential production of fatty liver, hepatitis, and cirrhosis in subhuman primates fed ethanol with adequate diets. Proc. Natl. Acad. Sel. USA, 72,437 - 441.
12.11.2004	(206)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-acute
Species	Rat
Sex	Male
Strain	Sprague-Dawley

Route of admin.	oral feed
Exposure period	4 week
Frequency of treatm.	Continuous
Post exposure period	None
Doses	Ethanol given in the diet at a concentration of 6% v/v to 30 rats.
Control group	Yes
NOAEL	
LOAEL	
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Cell proliferation (crypt cell production rate) was examinedin the gastrointestinal tract (oesophagus, stomach, duodenum, ileum, proximal colon and rectum) of 30 ethanol-treated rats and their pair-fed controls given an isocaloric liquid diet containing 36% total calories as either ethanol or carbohydrate. Blood samples were taken at the time of death.
Result	The crypt cell production rate was increased 2.1 fold in the rectal mucosa of treated rats ($p < 0.005$) but not in the other gut tissues examined. The proliferative compartment of the crypt was also expanded towards the colonic lumen in ethanol-treated rats ($p < 0.001$). Serum gastrin concentrations were significantly increased ($p < 0.01$). All tissues of the gastrointestinal tract were normal by light microscopy.
Reliability	(4) not assignable
Reference	Simanowski, UA et al. (1986) Chronic ethanol consumption selectively stimulates rectal cell proliferation in the rat. Gut 27, 278 - 282.
17.11.2004	(208)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-chronic
Species	Monkey
Sex	Male
Strain	Other
Route of admin.	Other
Exposure period	3 month
Frequency of treatm.	twice daily
Post exposure period	None
Doses	Ethanol comprised 40% of the ingested calories in a group of 14 animals.
Control group	Yes
NOAEL	

LOAEL	
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	A dose level in g/kg body weight can not be derived from theinformation presented in the report of this study. Fourteen rhesus monkeys were given a nutritionally adequate liquid diet containing 40% of the total calories as alcohol,twice a day by gavage for 3 months. A control group of 12 monkeys received the same diet, with the ethanol replaced bycarbohydrate. At the end of the study, a complete necropsy was performed, and an unspecified range of tissues was examined microscopically.
Result	The treatment had no effect on body weight gain. Marked accumulation of triglycerides, cholesterol and phospholipids occurred in the serum and liver. Although generalized fatty change was evident in the liver, cirrhosis did not develop. The relative heart weight was increased and microscopic effects on the heart were observed (fatty change in the myocardium, focal myocytolysis, atrophy of muscle bundles and early fibrosis). Triglyceride and cholesterol ester levels were increased in the heart. ECGs were normal. There were no effects on haematological parameters or gross or microscopic effects on the pancreas, kidneys, spleen or lungs.
Reliability	(4) not assignable
Reference	Vasdev, S.C. et al. (1975) Myocardial lesions induced by prolonged alcohol feeding in rhesus monkeys. Cardiovascular Res. 9, 134 -140.
12.11.2004	(212)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-acute
Species	Rat
Sex	Male
Strain	Sprague-Dawley
Route of admin.	Gavage
Exposure period	Up to 10 weeks
Frequency of treatm.	Daily
Post exposure period	None
Doses	5 g/kg body weight/day given to groups of 4 or 6 rats.
Control group	Yes
NOAEL	
LOAEL	
Method	other

Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Groups of 4 rats were treated with ethanol daily for 0, 1, 2, 5 or 10 weeks, and then given a final dose of 5 g ethanol/kg body weight 3 hours prior to being killed. The livers were removed and the mitochondria and microsomes wereexamined for evidence of diene conjugation (a method for detecting lipid peroxidation). Further groups of six rats were treated daily for 0, 1, 2, 3, 5 or 7 weeks prior to being killed. The livers were thenremoved and enzyme activities determined.
Result	Control rats. were given isocaloric sucrose in both cases. Mitochondrial lipid peroxidation was increased in 2 of 4 rats at week 0 (I.e. after an acute dose of ethanol but withno pre-treatment), 3 of 4 rats after t week of ethanol treatment, and in all treated rats from week 2 onwards. Microsomal peroxidation was not seen at week 0, but was evident in treated rats from 2 weeks onwards. The activities of hepatic glutathione peroxidase and glutathione reductase were increased by ca. 45 and 14% respectively at all time points.
Reliability	(4) not assignable
Reference	MacDonald, C.M. (1973) The effects of ethanol on hepatic lipid peroxidation and on the activlties of glutathione reductase and peroxidase. FEBS Letters 35, 227 - 230.
12.11.2004	(213)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-acute
Species	Rat
Sex	Male
Strain	Sprague-Dawley
Route of admin.	Inhalation
Exposure period	14 days
Frequency of treatm.	Continuous
Post exposure period	
Doses	10mg/l for 3 days then 25mg/l
Control group	yes, concurrent no treatment
NOAEL	
LOAEL	
Method	other
Year	1988

GLP	no data
Test substance	ethanol (64-17-5)
Remark	Study designed to assess the effects of ethanol on immune and hematopoietic systems. Full method details provided in reference.
Result	Ethanol blood levels measured at 169 +/-14 mg %. No weight changes were observed. A decrease in cellularity was found in the spleen, thymus and bone marrow. Red and white blood cell counts and haemoglobin concentration were not affected. Ethanol treatment did alter the relative proportions of lymphocytes and polymorphonuclear leukocytes in the peripheral blood. In the bone marrow, granulocyte macrophage progenitor cells were not affected but there was a decline in erythroid progenllor cells. The proliferation ability of splenic lymphocytes when stimulated by mitogens was unaffected.
Test Substance	95% ethanol.
Reliability	(4) not assignable
Reference	Marietta CA, Jerrells TR. Meagher RC, Karanian JW, Weight FF, Eckardt MJ (1988) Effects of long term ethanol inhalation on the immune and hematopoetic systems of the rat, Alcoholism 12 (2) 211-4.
18.11.2004	(214)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-acute
Species	Rat
Sex	Male
Strain	Sprague-Dawley
Route of admin.	Inhalation
Exposure period	3, 6, 9, 26 day groups
Frequency of treatm.	Continuous
Post exposure period	
Doses	20mg/l
Control group	Other
NOAEL	
LOAEL	
Method	other
Year	1979
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Full details provided in reference. Additional set of animals treated sub-cutaneously daily with pyrazole and a control set treated with saline.

	Ethanol levels assayed twice daily and in triplicate. Blood ethanol levels measured in duplicate by gas chromatography details of method provided in reference. Also measured: - plasma retention of sodium sulfobromopthalein - Plasma activity of glutamic pyruvic transaminase and - glutamic oxalacetic transaminase - Liver triglycerides - Phagocytic function ~ Liver and spleen histopathology. Statistical analysis by student's t test.
Result	Whilst a well reported study, the results are of limited value in assessing the toxic properties of ethanol relevant to its use as a chemical substance. Ethanol exposure produced a small but noticeable retardation in bodyweight gain. Initial exposure produced lethargy, ataxia and intoxication but animals adapted and appeared normal at the end of the study. Blood ethanoUevels in the ethanol-saline group peaked on day 9 at 126+/40mg/100ml and declined by day 26. In the ethanol-pyrazole group they peaked at 219mg/1 DOml (+/- 35). No blood ethanol was measured in either the air-saline or air-pyrazole controls.. Liver triglycerides were raised (doubled) for the ethanol groups at the earlier time points but were the same as the controls by day 26. Plasma triglycerides showed no consistent pattern. Plasma glutamic pyruvic transaminase levels were raised by 20% in the ethanol-saline group compared to the control. Liver samples from the ethanol-saline group exhibited mild vacuolisation for the early time periods, but this was not seen at 26 days. No other parameters were significantly effected between the ethanol-saline and air-saline groups.
Reliability	(2) valid with restrictions
Reference	Di Luzio NR, StegeTE (1979) Influence of chronic ethanol vapour inhalation on hepatic parenchymal and Kupffer cell function. Alcoholism: Clin Exp Res 3 (3) 240.
17.11.2004	(215)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-acute
Species	Rat
Sex	Male
Strain	Sprague-Dawley
Route of admin.	Inhalation
Exposure period	35 days
Frequency of treatm.	Continuous

Post exposure period	
Doses	see method details
Control group	yes, concurrent no treatment
NOAEL	
LOAEL	
Method	other
Year	1990
GLP	no data
Test substance	ethanol (64-17-5)

Method	Detailed method provided in reference. Ethanol vapour concentration adjusted to maintain a blood ethanol level of 200-300mg/dl (sufficient to produce signs of intoxication and ataxia levels 2-3 as defined by Majchrowijz(1975). Rats sacrificed within t hour of exposure, lungs and livers removed, weighed and snap frozen in liquid nitrogen. Blood ethanol levels determined (method provided in reference). Liver and lung glutathione and malonaldehyde levels measured (method details provided.) Enzyme assays also carried out and vitamin E levels measured.
Result	Ethanol exposed rats showed retarded weight gain. Lung and liver weights not affected but a moderate decrease in hepatic total protein and a small decrease in pulmonary soluble protein observed with ethanol exposure. Ethanol did not affect levels of glutathione of vitamin E in the lung but levels were significantly diminished in the liver. However, this change disappeared if levels expressed per gram of protein. Ethanol had no effect on malondialdehyde levels in either tissue.. Of the enzymes, catalase and superoxide dismutase levels were significantly increased in the lung by ethanol exposure. Other enzyme levels (glutathione peroxidase and reductase) were not affected. There was no effect on anti-oxidant enzyme levels in the liver.
Conclusion	Ethanol exposure does not produce a significant degree in oxidative stress in rat lung.
Reliability	(4) not assignable
Reference	Rikans, LE, Gonzalez LP (1990) Antioxidant protection systems of rat lung after chronic ethanol inhalation, Alcoholism: Clin Exp Res, 14 (6) 872-7.
17.11.2004	(216)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-acute
Species	Rat
Sex	Male

Strain	Other
Route of admin.	oral feed
Exposure period	3 to 4 weeks (not further defined)
Frequency of treatm.	Continuous
Post exposure period	no data
Doses	ethanol consumed by groups of 12 rats equivalent to 12.1 to 16.9 g/kg body weight/day
Control group	Yes
NOAEL	
LOAEL	
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Remark	In the first experiment, rats received 36% of their total calories as either ethanol or isocaloric dextrin maltose. In the second experiment, they received 36% of their calorific intake as ethanol or isocaloric fat. The ethanol was administered in a liquid diet at 5 g/100 ml diet. At the end of the study, the small intestine was removed for examination. Strain: CD
Result	Reduced body weight gain was seen in the ethanol-treated rats regardless of whether ethanol was substituted for carbohydrate or fat ($p < 0.01$). There was no effect on small intestine weight. The intestinal villi were shorter and contained fewer cells in the treated rats ($p < 0.001$), but showed no haemorrhagic erosions. Effects on the crypts indicative of cellular proliferation were seen (increased epithelial cell count and mitotic index, increased thymidine kinase activity and higher incorporation of tritiated thymidine into intestinal DNA).
Reliability	(4) not assignable
Reference	Baraona, E. et al. (1974) Small intestinal damage and changes in cell population produced by ethanol ingestion in the rat. Gastroenterology, 66, 226 - 234.
12.11.2004	(217)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sub-acute
Species	Mouse
Sex	Female
Strain	C57BL
Route of admin.	Inhalation
Exposure period	20-43 days
Frequency of treatm.	Continously

Post exposure period	
Doses	10-25mg/l
Control group	yes, concurrent no treatment
NOAEL	
LOAEL	
Method	other
Year	1986
GLP	ethanol (64-17-5)
Test substance	
Method	Animals 12-24 weeks old. Caged mice placed in perspex inhalation chambers. Feed: CRM pellets (K&K Greefe), freely available during exposure. Aged matched control mice used Blood obtained in heparinised syringes (cardiac puncture) then mixed with EDTA. Hb, RBC and WBC determined by Coulter counter. PVC measured using microhaematocrit tubes. Platelet count determined (after 100x dilution in formal citrate) using a Neubauer counting chamber. Reticulocytes counted on unfixed smears of supervitally -stained blood. Blood films stained by the May-Grunwald-Giemsa method and differential leucocyte counts performed on 500 consecutive nucleated cells. Femoral marrow expekked into heparinised Hank's solution, dispersed into a single cell suspension and used for determination of marrow cellularity or deoxyuridine suppression values. Quantification of granulocyte-macrophage progenitor cells: Femoral marrow expelled into MEM alpha medium. Samples dispersed into single cell medium, washed twice, assays of CFU-GM performed on each marrow cell suspension in triplicate. Details of procedure given in reference.
Result	Mice exposed to ethanol developed thrombocytopenia only and none of the more extensive effects seen following short exposure to higher concentrations. There was no effect on bone marrow. Effects are only believed to occur following exposures >22-24mg/l
Reliability	(4) not assignable
Reference	Malik F, Wickramasinghe (1986) Haematological abnormalities in mice continuously exposed to ethanol vapour. Br J. Exp. Path. 67, 831-8
17.11.2004	(181)

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Species:	rat
Strain:	Sprague-Dawley (SD)

Sex:	male and female
Route of Admin.:	inhalation
Exposure Period:	13 weeks
Freq. of Treatment:	6 h/day, 5 days/week 65 exposure days (13 weeks)
Post Exposure Observation Period:	N/A
Doses:	0, 500, 1500, and 3000 ppm
Control Group:	yes
NOAEL:	500 ppm
LOAEL:	1500 ppm
Method:	Conducted according to the US EPA Toxic Substances Control Act Health Effects Testing Guidelines:40 CFR 798.2450, Inhalation Toxicology (with the exception that the tissues from the central and peripheral nervous systems were not examined histologically. A histological examination of the central and peripheral nervous systems from the companion neurotoxicity study was conducted. Male and female Sprague-Dawley (SD) rats were exposed to concentrations of 0, 500, 1500, or 3000 ppm of n-butyl acetate for at least 65 exposures over 14 weeks. The animals were exposed in 4200 L glass and stainless steel chambers for 6 hours per day. Metering the liquid test substance through heated glass distillation columns packed with glass beads generated vapors of the test substance. The timeweighted average analytical concentrations were within 10% of the target concentrations. The target analytical concentration for the 500-ppm group was increased to 550 ppm after consultation with the Sponsor because determination of chamber atmosphere homogeneity showed that the variation in actual exposure concentration at various locations in the chamber was on average 13% lower than the reference point. Animals were observed for signs of toxicity prior to exposure, once per hour during exposure, and 30 minutes to one hour after exposure. Body weights and feed consumption data were measured weekly throughout the study. Blood was collected from 5 animals per group after 30 days of exposure (these animals were then discarded), and from 10 animals per group at termination. Clinical chemistry and hematology parameters were determined on all blood samples collected. Ophthalmic exams were conducted on all animals prior to study start. During the last week of exposure, animals from the control and high-concentration groups were re-examined. Since no changes were. detected in the eyes of the high-concentration animals, the animals from the low- and mid-concentration groups were not re-examined. The animals killed after 93-94 days on study were necropsied, examined for gross lesions and tissues saved for histopathological examination. Terminal body weights and

selected organ weights were collected from the animals killed on study days 93-94.

Year: 1996

GLP: yes

Test substance: n-butyl acetate (>99.9% pure)

Remark: No spontaneous mortality occurred during the study. Animals were observed for signs of toxicity prior to exposure, once per hour during exposure, and 30 minutes to one hour after exposure.

Results: No spontaneous mortality occurred during the study. Animals exposed to 3000 ppm had reduced activity levels during exposure that were of generally minor severity. Signs of sialorrhea and red discoloration on the chin hair were also observed. Animals exposed to 1500 ppm exhibited reduced activity during exposure of generally minimal severity. Control and 500 ppm animals appeared normal during exposure. After exposure, animals in all groups had porphyrin nasal discharges and dried porphyrin stains around the nose. These clinical signs were occasionally seen during the morning examination before exposure. Mean body weights for the 3000 ppm groups were significantly lower than the control group throughout the study.
Overall weight gains for the 3000 ppm group were 62 and 78% of weight gains for the control group (males and females, respectively). Mean feed consumption for the 3000 ppm groups was significantly lower than for the control group throughout the study. Mean weekly feed consumption values for the 3000 ppm groups were 14-25% lower than the control group for male rats and were 6-16% lower than the control group for female rats.
Mean body weights for the 1500 ppm groups were significantly lower than the control group at certain times during the study. Overall weight gains were 90 and 107% of the control group (males and females, respectively). Mean feed consumption values for the 1500 ppm groups were significantly lower than for the control group throughout the study. Mean weekly feed consumption values for the 1500 ppm groups were 4-17% lower than the control group for male rats and were 1015% lower than the control group for female rats. Mean body weights for the 500 ppm groups were comparable to the control group throughout the study. However, mean feed consumption values for the 500 ppm groups were significantly lower than for the control group on several days throughout the study. Mean weekly feed consumption values for the 500 ppm groups were 3-12% lower than the control group for male rats and were from
2% higher to 7% lower than the control group for female rats.
No biologically significant differences in hematologic parameters were seen after 30 days or 90 days of exposure. No biologically significant differences in serum chemistries were observed among

groups. No treatment-related ophthalmologic changes were observed. Mean terminal body weights were significantly lower for the 1500 and 3000 ppm male and female groups compared with the control group. Organ weight changes independent of the body weight changes (noted above) were slight and limited to lower spleen weights in the male 3000 ppm group, higher testes weights in the male 1500 and 3000 ppm groups, higher lung weights for the 3000 ppm male group, and higher adrenal gland weights for the 1500 ppm female and 3000 ppm male and female groups. Signs of necrosis of the olfactory epithelium in some 1500 and 3000-ppm rats represent a localized, site-of-contact effect due to n-butyl ac tate. No other lesions were. observed microscopically that were considered to be compound-related. There was no effect on either epididymidal or testicular sperm counts.

Comments: The rapid in vivo hydrolysis of n-butyl acetate to 1-butanol makes this study directly applicable to 1-butanol exposures.
The NOAEL for systemic effects and the NOAEL for neurotoxicity can be calculated for I-butanol after corrections for molecular weight. These values would be 221 ppm and 1,300 ppm, respectively.

Reference: David, R.M., T. R. Tyler, R.E. Ouellette, W. D. Faber, and M. I. Banton. Evaluation of Subchronic Toxicity of n-Butyl Acetate Vapor. Accepted for publication, Food Chemical Toxicology, 39: 877-886.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Species: rat
Strain: Sprague-Dawley (SD)
Sex: male and female
Route of Admin. : inhalation
Exposure Period: 13 weeks
Freq. of Treatment: 6 h/day, 5 days/week 65 exposure days (13 weeks)
Post Exposure Observation Period: 2 weeks
Doses: 0, 500, 1500, and 3000 ppm
Control Group: yes
NOAEL: 3000 ppm
LOAEL: N/A
Method: The study consisted of two sets of animals, male and female ad libitum-fed Sprague-Dawley (SD) rats designated for functional observational battery, motor activity, and neuropathology endpoints (FOB/MAlNP) and male (3D) rats restricted to 12-14 g of feed per day and which were designated for schedulecontrolled operant behavior (SCOB). Both sets of animals were exposed to

concentrations of 0, 500, 1500, or 3000 ppm of nbutyl acetate for at least 65 exposures over 14 weeks. The animals were exposed in 4200 L glass and stainless steel chambers for 6 hours per day. Metering the liquid test substance through heated glass distillation columns packed with glass beads generated vapors of the test substance. The timeweighted average analytical concentrations were within 10% of the target concentrations. The target analytical concentration for the 500-ppm group was increased to 550 ppm after consultation with the Sponsor because determination of chamber atmosphere homogeneity showed that the variation in actual exposure concentration at various locations in the chamber was on average 13% lower than the reference point.
Animals were observed for signs of toxicity prior to exposure, once per hour during exposure, and 30 minutes to one hour after exposure. Body weights were collected weekly. Feed consumption data was not collected on the ad libitum-fed animals. At the end of the 14-week exposure period, five male and five female animals from the FOB/MA/NP groups were randomly selected and perfused systemically for neuropathologic examination. Brain, spinal cord swellings (with dorsal and ventral routes), dorsal root ganglia, sciatic nerve, and tibial nerves. were examined microscopically.

Year: 1996

GLP: yes

Test substance: n-butyl acetate (>99.9% pure)

Remark: The SCOB testing paradigm involved both fixed-interval (FI) and fixed-ratio (FR) schedules.

Results: NOAEL Neurotoxicity 3000 ppm
Animals exposed to 1500 or 3000 ppm had minimal to minor reduced activity levels. There was no evidence of a cumulative effect of exposure on the severity of reduced activity. There was. no evidence of a cumulative effect of exposure on the severity of reduced activity. Control and 500 ppm animals appeared normal during exposure. There were. no other apparent differences in the clinical condition of FOB/MA/NP and SCOB animals. Body weights andlor body weight gains were reduced in the 1500 and 3000-ppm male and female animals. No differences in body weight or rate of weight gain were noted in the 500-ppm exposure group animals when compared to. control groups. There was no evidence of neurotoxicity based on FOB, motor activity, neuropathology, and SCOB endpoints.
Therefore, the no-observable effect level (NOAEL) for subchronic neurotoxicity for this study is 3000 ppm based on the lack of cumulative neurotoxicity following repeated exposure.

Comments: The rapid in vivo hydrolysis of n-butyl acetate to 1-butanol makes this study directly applicable to 1-butanol exposures.

References: David, R.M., Tyler, T.R., Ouellette, R.E., Faber, W.D., Banton, M.L, Garman, R.H., Gill, M.W., and O'Donoghue, J.L. . Evaluation Of Subchronic Neurotoxicity of N-Butyl Acetate Vapor. NeuroToxicology 19: 809-822, 1998.

Bernard, L.G., David, R.M., and Hosenfeld. 1996 A ThirteenWeek Subchronic Inhalation Neurotoxicity Study in the Rat. HAEL NO. 94-0305 and 94-0306, KAN 900710, CAS 00012386-4. Final Report. Toxicological Sciences Laboratory, Health and Environmental Laboratories Eastman Kodak Company Rochester, New York.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol

Test species/strain: male and female CD rats

Test method: SOP for Toxicity Research Laboratories. Four groups of male and female rats (30/sex/group) were dosed daily by gavage with 0,30, 125 or 500 mg/kg/day of 1-butanol for 13 weeks. Dosing solutions of butanol in deionized water were used and 10 mL/kg was the constant dosing volume. Body weights and feed consumption were recorded weekly. Clinical signs were recorded daily. Blood and urine were collected for clinical pathology at pre-dose (10 sentinel animals), and at the 13-week necropsies. Organ weights and results of gross pathology exams. were. recorded at the 13-week necropsies.
Histopathological examinations of tissues from the control and 1000 mg/kg groups were conducted.

GLP: Yes

Test results: Four groups of male and female rats (30/sex/group) were dosed daily by gavage with 0, 30, 125 or 500 mg/kg/day of 1-butanol for 13 weeks. There were no dose-related differences observed between treatment or control rats. on body or organ weight changes, food consumption or mortality. In addition, there were no dose-related differences observed in gross or histopathological examination of the eye. Ataxia and hypoactivity were observed in both sexes of the high dose group (500/mg/kg/day) during the final six weeks of the dosing period. The appearance of post dosing ataxia and hypoactivity only after the interim sacrifice suggests that, with the reduced number of animals, technicians were able to do more thorough observations in a shorter time frame. It is likely that the post dosing effects simply went unnoticed during the first half of the study. No treatment related signs were observed in the 30 or 125 mg/kg/day treatment groups.

Dose or concentration at which no toxic effects were observed: NOAEL: 125 mg/kg/day LOAEL: 500 mg/kg/day

Reference: Rat Oral Sub chronic Toxicity Study of Normal Butanol Toxicity Research Laboratories, Ltd. Muskegon, MI. TRL Study #032-006 dated 1986.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Test species/strain: Adult Male Long-Evans Rats
Test Method: Exposed to 4000 ppm (6 hours/day for 5 days, N = 10/group). Tested for auditory function 5 to 8 weeks post exposure using reflex modification audiometry (RMA).
Test Results: No change in hearing following exposure to n-butanol under these conditions.
GLP: No

Comments: These data contradict the results of a poorly-conducted human study (reported elsewhere in this document).
Reference: Crofton, K.M., Lassiter, T.L., and Rebert, C.S. 1994. Solvent induced ototoxicity in rats: an atypical selective mid-frequency hearing deficit. Hearing Research 80 (1), 25-30.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-butanol
Test species/strain: Rabbit
Test Method: Not Stated
GLP: No

Test Results: Dermal application of 42 to 55 ml/kg/day for 1 to 4 consecutive days to rabbits resulted in 100 percent mortality. Repeated applications to rabbits of 20 ml/kg/day for 30 days over a period of 6 weeks produced no fatalities.
Comments:

20 ml/kg = 16.20 g/kg = 16200 mg/kg
42 ml/kg = 34.02 g/kg = 34020 mg/kg
55ml/kg = 44.55 g/kg = 44550 mg/kg

Reference: Patty, F .A. 1982, Industrial hygiene and toxicology, 3rd ed., New York, Chichester, Brisbane, Toronto, Singapore, WileyInterscience. IIC: 4571-4578. As cited in World Health Organization (WHO). 1987. Environmental Health Criteria 65: Butanols Four Isomers: 1-Butanol, 2-Butanol, tert-Butanol,

Isobutanol. WHO,

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: Sub-chronic
Species: other: Albino rats **Sex:** male/female
Strain: other: ex Charles River
Route of administration: oral feed
Exposure period: 13 weeks
Frequency of treatment: daily
Post exposure period: none
Doses: 0.25% & 0.50% for 13 weeks; 1.0% for 10 weeks then 2.0% (week 11), 4.0% (week 12) and 6.0% (week 13).
Control Group: yes, concurrent no treatment
NOAEL: = 1127 mg/kg bw

Method: other: (see text)
Year: 1966
GLP: no
Test substance: as >95% 1-hexanol (111-27-3)

Remark: These results were reported to USEPA in accordance with TSCA 8(e).
Result: NOAEL (NOEL): M 1127 mg/kg/day F 1243 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0.25% M 182 mg/kg/day; F 216 mg/kg/day
0.5% M 374 mg/kg/day; F 427 mg/kg/day
1% M 1127 mg/kg/day; F 1243 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: One male at the lowest dose level (0.25%) died in the 9th week of the study. This was not attributed to treatment.
- Clinical signs: all surviving animals appeared normal.
- Body weight: comparable to controls.
- Food consumption: with the exception of high dose females at week 13 food consumption was comparable with that of controls. At week 13 female food consumption was 87.8% of control females at this time period. At this stage of the study the top dose level had been increased incrementally from 1% at week 10 to 6% in the diet at week 13.
- Clinical chemistry: not carried out.
- Haematology: No treatment related changes.
- Urinalysis: No treatment related changes.
- Organ weights: The original report indicates that there were

significant differences in some relative organ weights from treated groups compared to controls. These were reanalysed by the Weinberg Group using the Tukey test which indicated that only the increased heart weight in mid dose males remained significant. The significant changes found in the original report together with the results of the Weinberg analysis are summarised below.

Organ	Sex	Orig sig.	Weinberg report
Heart	M	mid-dose	Significant
Spleen	M	high dose	Not significant
	F	high dose	Not significant
	F	low dose	Not significant
Gonads	M	all levels	Not significant

Additionally Weinberg reanalysed the organ weight data for the liver, kidney, adrenal, brain and thyroid none of which showed significant changes in the original statistical analysis.
There were no significant changes except in the thyroid weight which showed a significant increase in top dose males according to the Weinberg analysis.

Statistical results are not reported in detail, while individual animal data are reported means are not given. Using this data to calculate the mean and SD for the organ weight changes originally reported as significant (see table above) the magnitude of the changes is a follows:

Spleen weight mean relative:

	Control	Low	Mid	High
Males	0.185	0.175	0.19	0.199*
SD	0.044	0.008	0.028	0.047
Females	0.189	0.223*	0.189	0.217*
SD	0.018	0.036	0.01	0.02

Gonad weight mean relative:

	Control	Low	Mid	High
Males	0.793	0.809*	0.814*	0.804*
SD	0.062	0.007	0.079	0.075

Heart weight mean relative:

	Control	Low	Mid	High
Males	0.296	0.268	0.331*+	0.328
SD	0.005	0.002	0.074	0.041

*Significant using Chi square test as reported in original report. +Significant in Tukey test.

- Gross pathology: Unremarkable
- Histopathology: There were no treatment related histopathological changes in the control and top dose animals examined.

STATISTICAL RESULTS: Original organ weight analyses using the Chi square test were supplemented by Tukey tests carried out by the Weinberg group.

Source: Scientific Associates, Inc. 1966a.

Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS

- Age: Actual age not reported, described as young.
- Weight at study initiation: M 103.8 g; F 90.4 g
- Number of animals: 10M + 10F per test group, 20M + 20 F controls.

ADMINISTRATION / EXPOSURE

- Duration of test/exposure: 13 weeks
- Type of exposure: Dietary
- Post exposure period: None
- Vehicle: Diet
- Doses: 0.2, 0.5 and 1% in the diet. The 1% dose ws increased to 2% in week 11, 4% in week 12 and 6% in week 13.

CLINICAL OBSERVATIONS AND FREQUENCY:

- Clinical signs: Daily (5 days/week)
- Mortality: Daily (5 days/week)
- Body weight: Weekly
- Food consumption: Weekly
- Water consumption: Not recorded
- Ophthalmoscopic examination: Not carried out.
- Haematology: At 30 days and 90 days on 5M+5F. Micro haematocrit, Hb, total & differential leucocytes.
- Biochemistry: Not carried out.
- Urinalysis: At 30 days and 90 days on pooled samples from 5 rats of each sex.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):

- Macroscopic: Complete necropsy performed, organ weights measured were brain, thyroid, heart, liver, spleen, kidneys, adreanls and gonads.
- Microscopic: Tissues fixed: brain, thyroid, parathyroid,

heart, lung, liver, spleen, stomach, small & large intestine, pancreas, kidney, urinary bladder, adrenals, gonads, lymph node, bone, bone marrow, muscle. All tissues from 5M+5F high dose and control animals were examined.

STATISTICAL METHODS: The original report indicates that a Chi square test was carried out on the organ:bodyweight ratio. It is not clear what statistical methods were used (if they were) for body weights, food consumption & haematological parameters. Subsequently The Weinberg Group Inc. used Tukeys test to re-analyse the organ weight data.

Test substance: Tradename is Alfol 6. Sample supplied by the Continental Oil Co. Louisiana (1965).

Conclusion: The NOAEL for Alfol 6 in rats following 13 week dietary exposure is 1127 mg/kg for males and 1243 mg/kg (highest test doses) for females (highest test doses) based on a lack of toxicologically significant effects at any dose level. The significant increase in relative heart weight in mid-dose males was not dose related and not correlated with histopathological change and was therefore not considered biologically significant. This was the only organ weight effect which was significant using both Chi square and Tukeys test. There were no histopathological changes in any organ.

Reported in Iuclid 2000.

Reliability: (2) valid with restrictions
Study reasonably well documented, meets generally accepted scientific principles, acceptable for assessment of the limited parameters assessed.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3

Scientific Associates, Inc. 1966a. Exhibit II. Final report on thirteen-week subacute feeding of Alfol 6 and Alfol 16 to rats.

02-JAN-2006 (29) (60)

<u>1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)</u>

Type: Sub-chronic
Species: dog **Sex:** male/female
Strain: Beagle
Route of administration: other: dietary at 0.5 & 1% (low & mid dose), high dose 1000 mg/kg/day by capsule
Exposure period: 13 weeks

Frequency of treatment: daily for dietary administration, 6 days/week via capsules.
Post exposure period: none
Doses: 0.5, 1.0% w/w and 1000 mg/kg/day
Control Group: yes, concurrent no treatment
NOAEL: = 370 - 435 mg/kg bw
LOAEL: = 1000 mg/kg bw

Method: other: see test conditions
Year: 1966
GLP: no
Test substance: >95% 1-hexanol (111-27-3)

Remark: These results were reported to USEPA in accordance with TSCA 8(e).
Result: NOAEL (NOEL), LOAEL (LOEL): M 370 mg/kg/day; F 435 mg/kg/day (M+F 403 mg/kg/day); LOEL 1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0.5% M 199 F 190 mg/kg/day
1% M 370 F 435 mg/kg/day
Top dose 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: 1000 mg/kg both males died day 23 & 38. Both females died day 1 & day 38. Another female was included which survived the 13 week exposure period. All control, lower & mid dose animals survived the exposure period.

- Clinical signs: 1000 mg/kd/day signs seen in all dogs, at some stage during the dosing period, were salivation, emesis, mild excitation, ataxia, slight tremors and varying stages of anaesthesia (which preceded death in all animals which died). No specific clinical signs in lower dose or control animals.

- Body weight gain: No difference from control values for the low & mid dose groups.

- Food consumption: No difference from control values for the low & mid dose groups.

- Ophthalmoscopic examination: Not done
- Clinical chemistry, Haematology, Urinalysis: No apparent differences between treated and control groups.

- Organ weights: No difference from control values for the low & mid dose groups.

- Gross pathology: Lymph node hyperplasia in both control & treated animals considered due to roundworm infestation (despite routine deworming throughout the study). In all animals which died there was evidence that the dogs may have aspirated vomit while anaesthetised (as a result of exposure to Alfol 6), death resulting from respiratory crisis. There was evidence of food particles in the trachea and the respiratory system smelled of the test substance.

- Histopathology: In top dose (1000 mg/kg/day) animals and to a lesser extent in animals of the intermediate dose level there was evidence of gastro-intestinal irritation (mucosal hyperemia without ulceration or acute inflammatory reaction). The 2 high dose males (both died) showed testicular atrophy while one high dose female which died showed decreased oogenesis, the ovaries of the female which surived exposure to the high dose level appeared within normal limits. Other than gastro-intestinal irritation in mid dose animals there were no other treatment related hisptopathological changes in dogs receiving 0.5 or 1% Alfol 6 in the diet.

- Other: ECG's showed no differences between the initial pattern recorded and those seen at 3 or 13 weeks.

STATISTICAL RESULTS: Analysis not carried out. Subsequent analysis of the data using Tukeys Test indicates no significant differences in organ weight data.

Source: Scientific Associates, Inc. 1966b.

Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS

- Age: 5 months
- Weight at study initiation: M4.77-8.97 kg; F4.31-7.95 kg
- Number of animals: 2M+2F treated; 4M+5F controls

ADMINISTRATION / EXPOSURE

- Duration of test/exposure: 13 weeks
- Type of exposure: 0.5% and 1% in the diet (low and mid dose) daily, 1000 mg/kg/day as a gelatin capsule 6 days/week (high dose, dietary high dose was unpalatable).
- Post exposure period: None
- Vehicle: Diet, none for top dose level(gelatin capsule).
- Doses: 0.5 and 1% in diet, 1000 mg/kg by gelatin capsules.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily 5 days/week. Complete physical examination, body temperature, pulse rate, reflexes, mucous membranes, auscultation pretreatment, 3, 6 & 13 weeks. ECG

pretreatment, 3 and 13 weeks.
- Mortality: Daily (5 days/week?)
- Body weight: weekly
- Food consumption: weekly
- Water consumption: Not recorded.
- Ophthalmoscopic examination: Not recorded.
- Haematology: Total & differential leucocyte counts, Hb, haematocrit, erythrocyte sedimentation rate, prothrombin time measured pretreatment, 3, 6 and 13 weeks.
- Biochemistry: Plasma levels of glucose, total protein & albumin, albumin/globulin ratios, urea nitrogen measured pretreatment, 3, 6 and 13 weeks. Liver function assessed by BSP retention, alkaline phosphatase & ASAT at same time periods.
- Urinalysis: albumin, glucose, bilirubin, pH, vol. , specific gravity, microscopic examination of sediment, total nitrogen. Carried out pretreatemnt & at 3, 6 & 13 weeks.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: complete, organ weights determined for brain, thyroid, heart, liver, kidneys, adrenals, spleen, gonads.
- Microscopic: Brain, pituitary, sub-maxillary salivary gland, thyroid, parathyroid, heart, lung, liver, spleen, stomach (fundic & pyloric), small intestine (3 levels), large intestine, pancreas, gall bladder, kidney, urinary bladder, adrenal, gonads, lymph node (cervical & mesenteric), bone, bone marrow, muscle (striated). All fixed. Tissues from controls & high dose animals examined microscopically. Stomach & intestinal tissues from mid dose animals also examined plus any abnormal tissues identified at necropsy.

STATISTICAL METHODS: No statistical analysis reported in the original report. For the HPV program the results were analysed using Tukey's Test.

Test substance: Tradename Alfol 6.

Conclusion: The NOAEL for Alfol 6 is considered to be 370 mg/kg day for male dogs and 435 mg/kg/day for females (dietary administration). The treshold for irritation of the gastrointestinal tract was 190 mg/kg/day. High dose animals

showed evidence of testicular atrophy 2/2 or decreased oogenesis 1/2. These animals died during the study and the effects are attributed to the acute lethality of the test substance adminstered at 1000 mg/kg by capsule. There were no adverse effects on the gonads at the lower dose levels. The value of this study is limited by the small numbers of test animals and the toxicity of the high dose level.

Reported in Iuclid 2000.

Reliability: (2) valid with restrictions
This study has methodological deficiences, animal group size too small (only 2M+2F in test groups), no statistical analysis, high mortality in top dose level which was administered by capsule while lower dose levels were administered in the diet. Useful as supporting data.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3

Scientific Associates, Inc. 1966b. Exhibit III. Final report on thirteen-week subacute feeding in Beagle dogs of Alfol 6 and Alfol 16.

09-JAN-2006 (29) (61)

<u>1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)</u>

Type: Sub-acute
Species: rat **Sex:** male
Strain: Fischer 344
Route of administration: oral feed
Exposure period: 3 weeks
Frequency of treatment: continuous
Post exposure period: none
Doses: 2, 4 and 8%
Control Group: yes
NOAEL: > 8 %

Method: other
Year: 1978
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: 1-hexanol did not have any significant effect on relative liver to body weight, liver catalase, liver carnitine acetyl transferase or hepatic peroxisome proliferation or in serum lipids compared to the control group. Results were presented

for the 2% dietary level but the authors indicate that 1-hexanol was also tested at dose levels or 4 and 8% with no adverse effects. 2-ethyl hexyl alcohol at 2% produced statistically significant ($p<0.001$) increases in all the above parameters except body weight and a decrease in serum triglycerides and cholesterol. The results of the serum lipid determinations are reported in a later publication (Moody & Reddy, 1982)

Test condition: The purpose of this study was to investigate the effects of various plasiticisers including DEHP and related materials on hepatic peroxisome proliferation and associated changes in liver parameters. 1-hexanol was included for comparison.

A group of 5 male rats received 2% 1-hexanol in the diet for 3 weeks, an untreated group of 13 male rats served as controls. The rats, housed individually, weighed 150-180 grams at the start of the study.

At the end of the exposure period the rats were sacrificed and blood, drawn from the abdominal aorta, was used for measurement of serum cholesterol and triglycerides. Liver sections were taken for electron microscopy. Liver carnitine acetyl transferase and hepatic catalase were measured spectrophotometrically.

Statistically evaluation was made using the students t-test.

Results are presented for the dietary level of 2% however the authors indicate that 1-hexanol was tested at 4 and 8% (results not reported).

Conclusion: Administration of up to 8% 1-hexanol in the diet of male rats for a period of 3 weeks did not in increase peroxisome proliferation or affect serum triglycerides or cholesterol. Reported in Patty, 2001.

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Reference: Moody, D.E; Reddy, J.K. 1978 Hepatic peroxisome (microbody) proliferation in rat plasticizers and related compounds. Tox. Apl. Pharm. 45: 497-504, 1978.

Moody, D.E; Reddy, J.K. 1982 Serum triglyceride and cholesterol contents in male rats receiving diets containing plasticizers and analogues of the ester 2-ethylhexanol. Toxicol Letters 10: 39-383.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols
(Monohydric alcohols) John Wiley & Sons - on line.
15-JUL-2005 (38) (39) (48)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: Sub-chronic
Species: rabbit **Sex:**
Route of administration: inhalation
Exposure period: 6 months
Frequency of treatment: not reported
Doses: 28.3 ppm
Control Group: no data specified

Method: other: no data
Year: 1971
GLP: no
Test substance: other TS: described as hexanol but not specifically identified as 1-hexanol

Remark: Limited reporting of a 1971 Russian study in which electron microscopic examination of the retina of the eyes of rabbits exposed by inhalation to vapours of 118 mg/m3 (28.3 ppm) hexyl alcohol for 6 months revealed ultrastructural changes in the photoreceptor cells and Muller fibres. No further experimental details were available. While referred to in Patty 2001, the fuller report is to be found in Patty 1982. This study also appears to be reported in RTECS.
Reliability: (4) not assignable
Secondary literature. original reference in Russian and unobtainable.
Reference: Patty Industrial Hygiene and Toxicology, 1982, Clayton, G.D. and Clayton, F.E. (eds.). Rowe & McCollister Chapter 55 Alcohols. Patty's Vol. IIC. New York: John Wiley & Sons, Inc.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols
(Monohydric alcohols) John Wiley & Sons - on line.

RTECS, 2004
13-OCT-2004 (47) (48) (55)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: Sub-chronic
Species: rat **Sex:**

Strain: Sprague-Dawley
Route of administration: i.p.
Exposure period: 30 weeks
Frequency of treatment: Daily, 6 days/week
Post exposure period: None
Doses: 102.5 mg/kg/day
Control Group: yes, concurrent vehicle

Method: other
Year: 1978
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: This study was carried out to investigate the possible peripheral neurotoxicity of 1-hexanol (and 2-hexanol) known metabolites of the known peripheral neurotoxin n-hexane. 1-hexanol did not produce the typical EMG alterations observed with n-hexane and in particular the distal motor latency was unchanged. There were also no clear cut abnormalities of the peripheral nerve. The relevance of the decrease in sensory conduction velocity is unclear.

Test condition: Groups of male rats (10 controls, 20 treated) weighing 340-350 g, received a single ip dose of 1-hexanol (12.5% in peanut oil) daily 6, days/week for 30 weeks. Controls received the same volume of peanut oil (1 ml/kg) as the treated group.

The rats were examined clinically weekly. At 8 weeks and again at the end of the test period the rats were subjected to neurophysiological examinations (electromyograph).

Measurements were made of motor and sensory conduction velocity, sensory potential amplitude and distal motor latency.

After the neurophysiological examinations at the end of the study 2 rats from each group were sacrificed and the peripheral nerves were removed and examined after suitable treatment.

Dunnetts test was used to assess statistical significance.

Test substance: 1-hexanol >98% pure

Conclusion: This neurophysiological investigation in rats following long term exposure to 1-hexanol indicates that 1-hexanol (n-hexane metabolite) does not produce the the typical changes in EMG characteristic of peripheral neuropathy induced by n-hexane.

Reliability: (2) valid with restrictions

Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Reference: Perbellini L. et al 1978 an experimental study on the neurotoxicity of n-hexane metabolites: Hexanol-1 and hexanol-2.

29-SEP-2004 (49)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Remark: Secondary report of Russian language reference, 1988. This summary data reports effects in rats following repeated inhalational exposure to 180 mg/m3 decanol (isomers not specified), 4 hours/day for 137 days. Effects noted were degenerative changes to the brain and meninges, multiple effects on the liver and unspecified effects on the urinary system. Unspecified effects were reported on the sense organs following repeated inhalation exposure to 58 mg/m3 for 26 weeks.

From the same source information is provided of a rabbit inhalation study where 200 mg/m3, 2 hours/day for 30 days caused effects on the optic nerve together with corneal damage and an effect on true cholinesterase.

An additional secondary source for the rabbit study, reported by RTECS, is NTIS document PB 234-882, Scientific Literature Review of Aliphatic Primary Alcohols, Esters and Acids in Flavor Usage.

Test substance: Decanol (isomeric content not specified)

Reliability: (4) not assignable
Secondary reference, original not available.

Reference: RTECS on line 2004 Decyl Alcohol

14-SEP-2005 (74)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	oral feed
Exposure period	:	Males 41-45 days; Females aprox. 54 days
Frequency of treatment	:	continuous in the diet
Post obs. period	:	none
Doses	:	0, 1500, 7500 & 30,000 ppm (approx 100, 500, 2000 mg/kg bw/day)
Control group	:	yes

NOAEL	:	= 2000 mg/kg bw
Method	:	other: Draft OECD 422 Combined Repeat dose and Reproductive/Developmental Toxicity Screening Test.
Year	:	1992
GLP	:	yes
Test substance	:	dodecanol (112-53-8)
Test condition	:	TEST ORGANISMS - Age: 7 weeks - Number of animals: 12M+12F/group ADMINISTRATION / EXPOSURE - Duration of test/exposure: males: 41-44 days; females approx. 54 days - Type of exposure: Dietary - Post exposure period: None - Vehicle: Diet. Diet preparation involved first mixing an aqueous dodecanol solution with the barley component, which varied for each dose level. The other components of the diet were then added. CLINICAL OBSERVATIONS AND FREQUENCY: - Mortality: Daily - Body weight: weekly - Food consumption: weekly - Water consumption: ad lib - Haematology: Males only at day 37; haematocrit, Hb, total RBC & WBC and differential WBC. No indication as to whether animals were fasted prior to sampling. - Biochemistry: Males only at day 37; Plasma protein, alkaline phosphatase, AAT, glucose, urea, creatinine,total & free cholesterol and triglyceride. No indication as to whether animals were fasted prior to sampling. ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC): - Macroscopic: Full necrospy on all animals. - Organ weights: liver, kidneys, thymus (females) liver, kidney, thymus, testes, epididymes (male) - Microscopic: Carried out on all control and top dose animals plus any obvious lesions observed at necrospy. Organs examined were liver, kidneys, adrenals, brain, heart, spleen, ovaries or testes and epididymes. OTHER EXAMINATIONS: The results of foetal examinations and reproductive parameters are reported in the appropriate sections.

STATISTICAL METHODS: Using the SAS-stat program analysis of variance plus Dunnett's test if changes were significant.

Result : NOAEL 2000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
Males: 102.4, 530.8 and 2046.4 mg/kg/day (mean of values reported for 2 weeks prior to mating and 3 weeks after mating)
Females:130.5, 657.5 and 2870.5 mg/kg/day (mean of values reported 2 weeks prior to mating)
- Time of death: There were no mortalities in this study.

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: None
- Clinical signs: None reported
- Body weight gain: No differences between treated and controls of either sex.
- Food consumption/food efficiency: No differences between treated and controls of both sexes.
- Clinical chemistry: (males only investigated) There was a significant reduction in plasma triglyceride (TG) at the top dose level and a significant reduction in plasma free cholesterol (F-chol) at the intermediate dose level. The reduced cholesterol level was re-analysed after removing 2 outlying values when the statistical significance was lost. These results may have been confounded by the difference in dietary composition between groups.

	0	100	500	2000 mg/kg
T-chol	1.60	1.74	1.64	1.75
F-chol	0.18	0.16	0.11*	0.15
TG	0.58	0.42	0.45	0.31**

* P<0.05 ** P<0.01 T-chol Total cholesterol

- Haematology: (males only investigated) A dose related reduction in total WBC was observed which reached statistical significance in top and mid dose males, there were no differences in the differential white cell count which explained these observations. The mean white blood cell counts (mmol/l) for males were at 0, 100, 500 and 2000 mg/kg 7.0, 5.9, 4.3*** and 4.7** respectively. ** P<0.01 *** P<0.001

- Organ weights: There were no dose related changes in organ weights. In males only there was a reduction in relative and absolute liver weights at the low dose level and a reduction in relative liver weight at mid doses, the top dose was comparable to controls.

	0	100	500	2000 mg/kg
Abs liver wt	12.27	11.20*	11.76	11.98
Rel. liver wt	3.3	3.1*	3.1*	3.3

* P<0.05

- Gross pathology: There were no changes attributable to exposure to the test compound.
- Histopathology: There were no treatment related histopathological changes.

STATISTICAL RESULTS: reported above.

Conclusion : The NOAEL for systemic toxicity in male rats is considered to be 2000 mg/kg/day (highest dose tested) in the absence of toxicologically significant effects at any dose level. A reduction in white cell count in all treatment groups was considered of doubtful significance in the absence of any changes in the differential cell count (based on WBC the NOEL is <100 mg/kg/day). A reduction in triglyceride and cholesterol levels at the top dose level, while possibly indicative of mild liver effects, may have been confounded by differences in dietary composition.

Reliability : (2) valid with restrictions
Comparable to guideline study (draft guideline) with acceptable restrictions

Source : Hansen 1992a
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Hansen, E. 1992a. Combined repeat dose and reproductive/developmental toxicity screening test on 1-dodecanol in rats. Institut of Toxicology, Danish National Food Agency, IT 921105.

09.01.2006 (9)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)</u>

Remark: There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for tetradecanol, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A) and C16 (1-hexadecanol). The oral NOAELs for these studies are all in

excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.

Source: Hayes Consultancy Service Bromley, Kent
Test substance: > 95% 1-Tetradecanol (112-72-1)
Conclusion: Expected to be of low systemic toxicity on repeated exposure.
Reliability: (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
Reference: SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.
15-SEP-2005 (66) (78)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Type: Sub-acute
Species: rat **Sex:** male/female
Strain: Sprague-Dawley
Route of administration: gavage
Exposure period: 28 days
Frequency of treatment: daily, 5 days/week
Post exposure period: 28 days
Doses: 100, 500, and 1000 mg/kg bw
Control Group: yes, concurrent vehicle
NOAEL: > 1000 mg/kg bw

Method: other: similar to OECD Guide-line 407
Year: 1985
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: NOAEL: >1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0, 100, 500 and 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: None
- Clinical signs: Unremarkable other than top dose females appearing rather defensive when handled.
- Body weight gain: Comparable with controls.
- Food and water consumption: Similar to control group
- Ophthalmoscopic examination: Comparable in treated and control animals.

- Clinical chemistry: Statistically significant changes (*95% ** 99% confidence) in some clinical chemical parameters were noted as follows:
500 mg/kg/day males increased potassium*, 500 mg/kg/day females increased GGT*, cholesterol** and chloride*. Glucose was elevated in top dose males (1000 mg/kg/day)**. These changes were not dose and/or sex related and not correlated with any histopathological findings and are therefore not considered of toxicological significance.

Serum glucose mmol/l:

Control	Low	Mid	High
6.03	6.20	6.25	7.28**

- Haematology: No differences between treated and control animals other than an increase in neutrophils containing rodlike bodies observed in top dose females (confidence level 95%*). Values obtained (% rod like cells) were controls 2.5, low dose 3.3, mid dose 2.9, high dose 5.3*.

- Organ weights: Both absolute and relative organ weights were essentially comparable in treated and control animals. Sporadic changes were observed as follows (*95% ** 99% confidence) increases in absolute organ weight male kidney 500 mg/kg/day*, male testes 1000 mg/kg/day*. The only change in relative organ weight was an increase in male adrenal weight at 1000 mg/kg/day*.

Testes weight mean relative (absolute):

Control	Low	Mid	High
0.856	0.839	0.908	0.893
(3.207)	(3.186)	(3.455)	(3.474)*

Adrenal weight mean relative (absolute)

Control	Low	Mid	High
0.013	0.014	0.014	0.015*

(0.050) (0.054) (0.055) (0.058)

- Gross and Histopathology: No treatment related histopathological changes in test, control or reversibility groups.

Source: Henkel KGaA 1985a (in German); Henkel 1999 (a 1-page English summary).

Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS
- Age/Weight at study initiation: M 84-98 g; F 81-93g
- Number of animals: 10M+10F per dose level plus 5M+5F per dose level for reversibility.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 27-28 days exposure (5 days/week)
- Type of exposure: oral gavage
- Post exposure period: 28 days
- Vehicle: Olive oil
- Concentration in vehicle: 0, 2, 10 or 20%
- Total volume applied: 5 ml/kg
- Doses: 0, 100, 500 and 1000 mg/kg/day

SATELLITE GROUPS AND REASONS THEY WERE ADDED: 5M+5F per dose level for reversibility.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily
- Mortality: Daily
- Body weight: Weekly
- Food consumption: Daily
- Water consumption: Weekly
- Ophthalmoscopic examination: At end of study
- Haematology: After 21/22 daily doses: Haematocrit, MCV, Hb, RBC, WBC, Thrombocytes, differential white count.
- Biochemistry: After 21/22 daily doses: Serum Urea, creatinine, Na, K, calcium, alkaline phosphatase, ALAT, ASAT, GT, bilirubin, chloride, albumin, total protein, chloesterol.
- Urinalysis: Not done

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Yes
- Organs weights: thyroid, adrenals, thymus, kidney, spleen, heart, brain, testes, liver.
- Microscopic: All organs from the control and top dose animals were examined plus the animals from the reversibility study.

STATISTICAL METHODS: T-test. U-test for organ weights.
Test substance: Tradename Lanette 16
Conclusion: NOAEL is considered to be >1000 mg/kg/day based on lack of toxicologically significant treatment related effects at this dose level (top dose level). Sporadic statistically significant changes in some organ weights and clinical chemical parameters were observed but these were not associated with histopathological changes and were not considered of toxicological significance.

This study is also reported in summary in Iuclid 2000 for hexadecanol.
Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
Report in German language, English summary page.
Flag: Critical study for SIDS endpoint
Reference: Henkel KGaA. 1985a. Lanette 16: 28-Tage-Test mit wiederholter oraler Verabreichung an Ratten. November 1985. Report No. TBD 850499. With pathology report No. 840394.

Henkel KGaA. 1999. Hexadecanol: Evaluation of repeated dose oral toxicity. Unpublished data, English summary and evaluation of Henkel 1985a report No. TBD 850499.
03-JAN-2006 (41) (43)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Type: Sub-chronic
Species: other: Albino rats **Sex:** male/female
Strain: other: ex Charles River
Route of administration: oral feed
Exposure period: 13 weeks
Frequency of treatment: Daily
Post exposure period: none
Doses: 1% and 2.5% for 13 weeks, 5% for 10 weeks then 7.5% (week 11) and 10.0 % (weeks 12 & 13).
Control Group: yes
NOAEL: = 723 mg/kg bw

Method: other: see text
Year: 1966
GLP: no data
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: These results were reported to USEPA in accordance with TSCA

8(e).

Result: NOAEL: M 723 mg/kg/day F 875 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
1%: M 723 mg/kg/day; F875 mg/kg/day
2.5%: M1822 mg/kg, day; F 2064 mg/kg/day
5%: M 4257 mg/kg/day; F4567 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: All animals survived the 13 week treatment period.

- Clinical signs: all surviving animals appeared normal.

- Body weight: Significantly reduced (84.7 - 89.8% of controls) in top dose males for most study weeks, in mid dose females at weeks 4-13 and high dose females (81.7-89.7%) throughout the study. Changes were attributed at least in part to reduced food consumption and the high content of test material in the diet.

- Food consumption: Significantly reduced (76.4 - 89.2% of controls) in top dose males at weeks 1 and 12, in mid dose males at week 13, in mid dose females at week 1 and high dose females weeks 1 and 12 (79.1 - 89.9% of controls).

- Clinical chemistry: not carried out.
- Haematology: no treatment related changes.
- Urinalysis: no treatment related changes.

- Organ weights: The original report indicates that there were significant differences in some relative organ weights from treated groups compared to controls. These were reanalysed by the Weinberg Group using the Tukey test. The significant changes found in the original report together with the results of the Weinberg analysis are summarised below.

Organ	Sex	Orig. sig. at	Weinberg report
Brain	M	low-dose	Not significant
	M	high-dose	Significant
	F	mid dose	Significant
	F	high-dose	Significant
Heart	M	high-dose	Significant
	F	high-dose	Not significant
Liver	M	mid dose	Not significant

	M	high-dose	Significant
	F	low-dose	Not significant
	F	mid dose	Not significant
	F	high-dose	Significant
Spleen	F	mid dose	Not significant
	F	high-dose	Significant
Gonad	M	low-dose	Not significant
	M	high-dose	Significant

Additionally Weinberg reanalysed the organ weight data for the kidney and adrenal and thyroid which showed no significant changes from the original statistical analysis. The thyroid weight showed a significant increase in mid dose males only according to the Weinberg analysis.

Statistical results are not reported in detail, while individual animal data are reported means are not given. Using this data to calculate the mean and SD for the organ weight changes originally reported as significant (see table above) the magnitude of the changes is a follows:

Brain weight mean relative:

	Control	Low	Mid	High
Males	0.454	0.486*	0.497	0.523*+
SD	0.01	0.029	0.072	0.03
Female	0.646	0.692	0.795*+	0.797*+
SD	0.066	0.021	0.004	0.01

Heart weight mean relative:

	Control	Low	Mid	High
Males	0.296	0.286	0.323	0.293*
SD	0.005	0.028	0.039	0.014
Female	0.305	0.315	0.329	0.392*+
SD	0.023	0.008	0.054	0.025

Liver weight mean relative:

	Control	Low	Mid	High
Males	3.029	3.168	3.09*	3.756*+
SD	0.302	0.021	0.653	0.361
Female	3.466	3.549*	3.55*+	3.659*
SD	0.198	0.139	0.008	0.275

Spleen weight mean relative:

	Control	Low	Mid	High
Female	0.189	0.205	0.212*	0.233*+
SD	0.018	0.025	0.009	0.065

Gonad weight mean relative:

	Control	Low	Mid	High
Males	0.793	0.768*	0.787	0.902*+
SD	0.062	0.003	0.084	0.052

*Significant using Chi square test as reported in original report. +Significant in Tukey test.

- Gross pathology: Unremarkable
- Histopathology: There were no treatment related histopathological changes in the control and top dose animals examined (including testes & ovaries).

STATISTICAL RESULTS: Original organ weight analyses using the Chi square test were supplemented by Tukey tests carried out by the Weinberg group.

Source: Scientific Associates, Inc. 1966a.

Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS

- Age: Actual age not reported, described as young.
- Weight at study initiation: M 103.8 g; F 90.4 g
- Number of animals: 10M + 10F per test group, 20M + 20 F controls.

ADMINISTRATION / EXPOSURE

- Duration of test/exposure: 13 weeks
- Type of exposure: Dietary
- Post exposure period: None
- Vehicle: Diet
- Doses: 1.0, 2.5 and 5% in the diet. The 5% dose was increased to 7.5% in week 11 and 10% in weeks 12 and 13.

CLINICAL OBSERVATIONS AND FREQUENCY:

- Clinical signs: Daily (5 days/week)
- Mortality: Daily (5 days/week)
- Body weight: Weekly
- Food consumption: Weekly
- Water consumption: Not recorded
- Ophthalmoscopic examination: Not carried out.
- Haematology: At 30 days and 90 days on 5M+5F. Micro haematocrit, Hb, total & differential leucocytes.

- Biochemistry: Not carried out.
- Urinalysis: At 30 days and 90 days on pooled samples from 5 rats of each sex.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):

- Macroscopic: Complete necropsy performed, organ weights measured were brain, thyroid, heart, liver, spleen, kidneys, adrenals, ovaries & testes.
- Microscopic: Tissues fixed: brain, thyroid, parathyroid, heart, lung, liver, spleen, stomach, small & large intestine, pancreas, kidney, urinary bladder, adrenals, ovaries, testes, lymph node, bone, bone marrow, muscle. All tissues from 5M+5F high dose and control animals were examined.

STATISTICAL METHODS: The original report indicates that a Chi square test was carried out on the organ:bodyweight ratio. It is not clear what statistical methods were used (if they were) for body weights, food consumption & haematological parameters. Subsequently The Weinberg Group Inc. used Tukeys test to re-analyse the organ weight data.

Test substance: Tradename Alfol 16

Conclusion: The NOAEL for this 13 week dietary feeding study in rats is ca 750 mg/kg/day (males 723, females 875) based on reduced weight gain and food consumption. The toxicological significance of observed changes in organ weights, all in the absence of histopathological change, is questionable. Increased liver weights at higher dose levels may be indicative of a mild adaptive effect on the liver.

This study was also reported in summary in Iuclid 2000 for hexadecanol.

Reliability: (2) valid with restrictions

Valid with restrictions including lack of biochemical investigations and limited reporting of statistical findings. Study reasonably well documented, meets generally accepted scientific principles, acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Hexadecan-1-ol Cas# 36653-82-4

Scientific Associates, Inc. 1966a. Exhibit II. Final report on thirteen-week subacute feeding of Alfol 6 and Alfol 16 to rats.

03-JAN-2006 (50) (77)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Type: Sub-chronic
Species: dog **Sex:** male/female
Strain: Beagle
Route of administration: oral feed
Exposure period: 13 weeks
Frequency of treatment: daily
Post exposure period: none
Doses: 0.5, 1.0, and 3.0 % w/w
Control Group: yes, concurrent no treatment
NOAEL: > 1054 mg/kg bw

Method: other: (see text)
Year: 1966
GLP: no data
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: These results were reported to USEPA in accordance with TSCA 8(e).
Result: NOAEL (NOEL): M 1175 mg/kg/day; F 1054 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0.5% (M 208 mg/kg/day; F 186 mg/kd/day)
1% (M 502 mg/kg/day; F 374 mg/kg/day)
3% (M 1175 mg/kg/day; F 1054 mg/kg/day)

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: No animals died.
- Clinical signs: No specific clinical signs, all animals appeared normal and healthy throughout the study. This was suppported by the clinical examinations at weeks 3, 6 and 13 which were within normal limits.
- Body weight gain: Comparable in test and control groups.
- Food/water consumption: Comparable in test and control groups.
- Ophthalmoscopic examination: Not carried out.
- Clinical chemistry: No treatment related adverse effects for most parameters. Plasma ALAT levels were increased at all dose levels at 13 weeks only.
- Haematology: No adverse effects.
- Urinalysis: No adverse effects.
- Organ weights: These were within normal limits and comparable to controls. Tukeys test did not indicate any statistical differences (however sample size was small).
- Gross pathology: Lymph node hyperplasia in both control and treated animals was considered due to roundworm infestation (despite routine deworming throughout the study). There were

no treatment related findings.
- Histopathology: No treatment related changes.
- Other: ECG's showed no difference between the initial pattern recorded pretreatment and those seen at 3 and 13 weeks.
STATISTICAL RESULTS: There was no statistical analysis of the study data in the original report. Subsequent analysis of organ weights using Tukeys test did not reveal any statistical differences between treated and control animals. This analysis was carried out by The Weinberg Group Inc.

Source: Scientific Associates, Inc. 1966b.

Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS
- Age: 5 months
- Weight at study initiation: M4.77-8.63 kg; F5.45-7.49 kg
- Number of animals: 2M+2F treated; 4M+5F controls

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 13 weeks
- Type of exposure: dietary
- Post exposure period: None
- Vehicle: Diet
- Doses: 0.5, 1% and 3% in diet

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily 5 days/week. Complete physical examination, body temperature, pulse rate, reflexes, mucous membranes, auscultation pretreatment at 3, 6 & 13 weeks. ECG pretreatment, 3 and 13 weeks.
- Mortality: Daily
- Body weight: weekly
- Food consumption: weekly
- Water consumption: Not recorded.
- Ophthalmoscopic examination: Not recorded.
- Haematology: Total & differential leucocyte counts, Hb, haematocrit, erythrocyte sedimentation rate, prothrombin time measured pretreatmentand at 3, 6 and 13 weeks.
- Biochemistry: Plasma levels of glucose, total protein & albumin, albumin/globulin ratios, urea nitrogen measured pretreatment, 3, 6 and 13 weeks. Liver function assessed by BSP retention, alkaline phosphatase & SGOT at same time periods.
- Urinalysis: albumin, glucose, bilirubin, pH, vol. , specific gravity, microscopic examination of sediment, total nitrogen. Carried out pretreatemnt & at 3, 6 & 13 weeks.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: complete, organ weights determined for brain, thyroid, heart, liver, kidneys, adrenals, spleen, gonads.
- Microscopic: Brain, pituitary, sub-maxillary salivary gland, thyroid, parathyroid, heart, lung, liver, spleen, stomach (fundic & pyloric), small intestine (3 levels), large intestine, pancreas, gall bladder, kidney, urinary bladder, adrenal, gonads, lymph node (cervical & mesenteric), bone, bone marrow, muscle (striated). All fixed. Tissues from controls & high dose animals examined microscopically. Stomach & intestinal tissues from mid dose animals also examined plus any abnormal tissues identified at necropsy.
STATISTICAL METHODS: No statistical analysis reported in the original report. For the HPV program the results were analysed using Tukey's Test.

Test substance: This substance corresponds to CAS# 36653-82-4. Tradename is Alfol 16. Described as a white, wax-like solid. No other analytical details.
Tradename Alfol 16

Conclusion: The NOAEL for Alfol 16 following dietary administration is considered to be >1175 mg/kg/day for male dogs and >1054 mg/kg/day for females. This was the highest dose level tested (3% in diet). The elevated ALAT values seen at 13 weeks in most test animals at all dose levels were apparently not dose related or accompanied by histopathological liver change. Other markers of liver function appeared normal. This study was also reported in summary in Iuclid 2000 for hexadecanol.

Reliability: (2) valid with restrictions
Reliability 2 however there were methodological deficiencies, animal group size too small (2M + 2F in test groups), no statistical analysis in original study, subsequent analysis by The Weinberg Group Inc of limited relevance because of small group sizes.

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Hexadecan-1-ol Cas# 36653-82-4

Scientific Associates, Inc. 1966b. Exhibit III. Final report on thirteen-week subacute feeding in Beagle dogs of Alfol 6 and Alfol 16.
03-JAN-2006 (50) (78)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Remark: Summary report from NTIS publication (not available). Repeated

oral administration to dogs of 91 g/kg over a 12 week period resulted in tremors, ataxia and death. No further details available.

Test substance: hexadecanol, no further information

Reliability: (4) not assignable
Secondary reference.

Reference: RTECS, 2004

06-AUG-2005 (71)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	28 days
Frequency of treatment	:	daily, 5 days/week
Post obs. period	:	28 days
Doses	:	0, 100, 500, 1000 mg/kg in olive oil
Control group	:	yes, concurrent vehicle
NOAEL	:	= 1000 mg/kg bw
Method	:	OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year	:	1986
GLP	:	yes
Test substance	:	octadecanol (112-92-5)
Test substance	:	Tradename Lanette 18
Test condition	:	TEST ORGANISMS - Supplier: Charles River Wiga GmbH, Sulzburg - Age/Weight at study initiation: M64-97 g; F 62-99g - Number of animals: 10M+10F per dose level plus 5M+5F per dose level for reversibility. ADMINISTRATION / EXPOSURE - Duration of test/exposure: 27-28 days exposure (5 days/week) - Type of exposure: oral gavage - Post exposure period: 28 days - Vehicle: Olive oil - Concentration in vehicle: 0, 2, 10 or 20% - Total volume applied: 5 ml/kg - Doses: 0, 100, 500 and 1000 mg/kg/day SATELLITE GROUPS AND REASONS THEY WERE ADDED:

5M+5F per dose level for reversibility.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily
- Mortality: Daily
- Body weight: Weekly
- Food consumption: Weekly
- Water consumption: Ad lib
- Ophthalmoscopic examination: At end of study
- Haematology: After 21/22 daily doses: Haematocrit, MCV, Hb, RBC, WBC, Thrombocytes, differential white count.
- Biochemistry: After 21/22 daily doses: Serum Urea, creatinine, Na, K, calcium, alkaline phosphatase, ALAT, ASAT, GT, bilirubin, chloride, Albumin, total protein, chloesterol.
- Urinalysis: Not done

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Yes
- Organs weights: thyroid, adrenals, thymus, kidney, spleen, heart, brain, testes, liver.
- Microscopic: All organs from the control and top dose animals were examined plus the animals from the reversibility study.

STATISTICAL METHODS: T-test, organ weights U-test.

Result : NOAEL: 1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0, 100, 500 & 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: No mortalities.
- Clinical signs: Unremarkable.

- Body weight gain: Male bodyweight gain was reduced compared to controls, body weight gains were 95%, 91% and 82% of control values for low, mid and high dose levels respectively at the end of the study. This was attributed to a high mean control bodyweight in males and marked inhibition of bodyweight gain in one male in each of the high and mid dose levels.

- Food/water consumption: Water consumption was comparable in control and treated groups. Food consumption was slightly reduced in males (95% confidence).

- Ophthalmoscopic examination: No treatment related ocular lesions.

- Clinical chemistry: There were some statistically significant changes (p=0.05) in clinical chemical parameters in the top dose group. In males ASAT was increased (control mean 33 U/l; top dose 45.1); Na was also increased (control mean 143.1 mmol/l; top dose 144.4). Serum chloride was reduced (control mean 99.7 mmol/l; top dose 97.9). In females there was an increase in Na (control mean 142 mmol/l; top dose 143) and in phosphorous (control mean 1.99 mmol/l; top dose 21.9. These changes are not clearly dose related and apart from the slight increase in serum sodium do not appear in both sexes. There are no histopathological changes related to these changes which were considered chance observations and not indicative of a trend.

- Haematology: Treated and control groups were comparable. A slight increase (95% confidence *) in neutrophils with rod-like bodies (mid dose males), a marginal decrease in thrombocytes (top dose males) and eosinophils (top dose females) were not considered of biological significance.

Thrombocytes:

	Control	low	mid	high
male	633.9	619.9	583.9	511.9*

Eosinophils:

female	1.3	0.8	0.9	0.3**

- Urinalysis: Not done

- Organ weights: Sporadic changes in absolute or relative organ weights relative weights were not dose and/or sex related. There was no corresponding histopathological change. Relative heart weights were increased* in top dose males, Relative and absolute kidney weights were decreased* in mid-dose females, while other absolute organ weights were changed as follows:

Absolute mean spleen weight:

	Control	low	mid	high
male	0.706	0.651	0.585*	0,593*

Absolute mean thyroid weight:

	Control	low	mid	high
male	0.024	0.018**	0.02	0.018**

Absolute mean spleen weight:

	Control	low	mid	high
male	0.706	0.651	0.585*	0.593*

Relative mean heart weight:

	Control	low	mid	high
male	0.281	0.288	0.302	0.314*

- Pathology: There were no treatment related findings. Pathological changes observed were related to misdosing, respiratory infection or viral infection.

STATISTICAL RESULTS: T-test and U-test for organ weights.

Conclusion : The NOAEL for this study is considered to be >1000 mg/kg/day based on a lack of toxicologically significant effects. Statistically significant changes in some clinical chemical and haematological parameters and organ weights changes were not accompanied by histopathological changes and were either not dose related or appeared in only one sex. These effects are not considered of toxicological significance.

Reliability : (1) valid without restriction
Guideline study

Source : Henkel KGaA 1986a; Henkel 1999 (2-page English summary)

Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference

Henkel KGaA. 1986a. Lannette 18: 28-Tage-Test mit wiederholter oraler Verabreichung an Ratten. Report No. TBD 860071. Institut fur Toxikologie. With pathology report No. 840230.

Henkel KGaA. 1999. Octadecanol: Evaluation of repeated dose oral toxicity. Unpublished data, English summary and evaluation of Report No. TBD 860071.

04.01.2006 (13) (14)

<u>1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)</u>

Species : rat
Sex : male/female
Strain : Wistar
Route of admin. : oral feed
Exposure period : males 45 days; females ca 54 days
Frequency of treatment : continuous in diet

Post obs. period	:	none
Doses	:	0, 1500, 7500 or 30,000 ppm (ca 0, 100, 500, 2000 mg/kg/bw/day)
Control group	:	yes
NOAEL	:	= 2000 mg/kg bw
Method	:	other: Draft OECD 422 combined repeated dose and reproductive/developmental toxicity screening test
Year	:	1991
GLP	:	yes
Test substance	:	octadecanol (112-92-5)
Test condition	:	TEST ORGANISMS - Age: 7 weeks - Number of animals: 12M+12F/group ADMINISTRATION / EXPOSURE - Duration of test/exposure: males: 45 days; females approx. 54 days - Type of exposure: Dietary - Post exposure period: None - Vehicle: Diet. Diet preparation involved first mixing the octadecanol with the barley component, the proportion of which varied for each dose level. The other components of the diet were then added. CLINICAL OBSERVATIONS AND FREQUENCY: - Mortality: Daily - Body weight: weekly - Food consumption: weekly (except during mating) - Water consumption: ad lib - Haematology: Males only at day 37; haematocrit, Hb, total RBC & WBC and differential WBC. - Biochemistry: Males only at day 37; Plasma protein, alkaline phosphatase, AAT, glucose, urea, creatinine,total & free cholesterol and triglyceride. ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC): - Macroscopic: Full necrospy on all animals. - Organ weights: liver, kidneys, thymus (females) liver, kidney, thymus, testes, epididymes (males) - Microscopic: Carried out on all control and top dose animals plus any obvious lesions observed at necrospy. Organs examined were liver, kidneys, adrenals, brain, heart, spleen, ovaries or testes and epididymes. OTHER EXAMINATIONS: The results of foetal examinations and reproductive parameters are reported in the appropriate sections.

STATISTICAL METHODS: Using the SAS-stat program analysis of variance plus Dunnett's test if changes were significant.

Result : NOAEL 2000 mg/kg/day, LOEL: 100 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
Males: 99.25, 500.25 and 2146.5 mg/kg/day (mean of values reported for 2 weeks prior to mating and 3 weeks after mating)
Females:120, 625 and 2435.5 mg/kg/day (mean of values reported 2 weeks prior to mating)

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: There were no mortalities.
- Clinical signs: None reported.

- Body weight gain: There were no significant changes in body weight or body weight gain in the 3 weeks prior to mating for both sexes. Or in males after mating.

- Food consumption/efficiency: Food consumption was significantly increased in top dose males ($p<0.001$) and in mid dose females ($p<0.05$) at week 3. There were no other differences in food consumption or food conversion efficiency.

- Clinical chemistry: (males only examined) There were significant (but non-dose related) differences in free cholesterol (increased) and triglycerides (decreased) at all dose levels. Total cholesterol levels were not significantly increased. Plasma glucose was elevated with statistical significance in the low and mid-dose groups.

Parameter (mM)	Control	100	500	2000
Free chol	0.29	0.38**	0.37**	0.36*
Total chol	1.30	1.56	1.56	1.40
Triglycerides	0.78	0.42**	0.49*	0.46**
Glucose	6.8	7.8*	7.9*	7.6

* $p<0.05$ ** $P<0.01$

- Haematology: No statistically significant differences between treated and control groups (males only examined).
- Organ weights: There were no significant differences in absolute or relative organ weights in males or females.

- Gross pathology: Unremarkable no changes attributable to

treatment.
- Histopathology: Unremarkable no changes attributable to treatment.

- Other: The method of diet preparation resulted in different dietary content between the different treatment groups and controls.

STATISTICAL RESULTS: Reported above.

Conclusion : The only systemic effects seen in this study were significant changes in plasma free cholesterol, triglycerides and glucose. These changes occurred at all dose levels but were not dose related. Although the reduction in plasma triglycerides levels may be indicative of mild effects in the liver, the differences in the composition of the test diets may have confounded these results. The NOAEL can be considered to be 2000 mg/kg/day with a NOEL of 100 mg/kg/day.

Reliability : (2) valid with restrictions
comparable to guideline study (draft guideline) with acceptable restrictions

Source : Hansen 1992b.
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Hansen, E. 1992b. Combined repeat dose and reproductive/developmental toxicity screening test on 1-octadecanol in rats. Denmark: Institute of Toxicology, National Food Agency, IT 911130.

03.01.2006 (9)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Remark: There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C20 (eicosanol) alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for C16 (1-hexadecanol), C18 (octadecanol) and C20 (docosanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated

exposure.
Test substance: >= 90% 1-eicosanol (629-96-9)
Conclusion: Expected to be of low systemic toxicity on repeated exposure.
Reliability: (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
Reference: SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category.
15-SEP-2005 (18) (23)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Type: Sub-chronic
Species: rat **Sex:** male/female
Strain: other: CD
Route of administration: gavage
Exposure period: 26 weeks
Frequency of treatment: daily, 7 days/week
Post exposure period: No
Doses: 10, 100, 1000 mg/kg bw-day
Control Group: yes, concurrent vehicle
NOAEL: = 1000 mg/kg bw

Method: other: standard regulatory protocol
Year: 2000
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)

Result: NOAEL: 1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 10, 100 and 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: One male at 100 mg/kg/day died on day 25, microscopic examination revealed changes consistent with aspiration of test material due to mis-dosing. There were no treatment related deaths.

- Clinical signs: None
- Body weight gain: Comparable in test and control groups.
- Food consumption: Comparable between test and control groups as was food efficiency.
- Ophthalmoscopic examination: No treatment related changes.
- Clinical chemistry: No treatment related changes.
- Haematology: No treatment related changes.
- Urinalysis: No treatment related changes.
- Organ weights: No treatment related changes.
- Gross pathology: No treatment related changes.
- Histopathology: No treatment related changes.
- Other: Concentrations of behenyl alcohol in the blood were measured on day 1 and in weeks 13 and 26. Maximum mean plasma conc. (Cmax) was observed 1 hour after dosing in all males and most females. 24 hours after dosing plasma concentrations were below the limit of quantification (<10ng/ml) at the 10 and 100 mg/kg dose levels while levels following administration of 1000 mg/kg/day remained quantifiable on each sampling day. Statistically significant differences in area under the curve (AUC24) were observed between males and females treated with 10 and 1000 mg/kg/day on day 1 and during week 13. The rate and extent of systemic exposure to rats as shown by AUC24 and Cmax on day 1 and in weeks 13 and 26 increased with increasing dose level. Increases were less than the proportionate dose increment and there was statistically significant evidence of non-proportionality on each sampling day.
STATISTICAL RESULTS: No statistically significant changes were observed in any of the parameters examined in the main study, the full results were therefore not presented in the publication. Statistical significance for monocytes, basophils, eosinophils and large unstained cell counts were not reported as these data were not normally distributed.

Source: Iglesias, 2002a

Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS
- Age: 28-35 days
- Number of animals: 20M+20F per treated and control groups

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 26 weeks
- Type of exposure: Oral gavage, daily 7 days/week
- Post exposure period: No
- Vehicle: 1% aqueous Tween 80.
- Concentration in vehicle: 20% stock suspension for top dose diluted to give standard volume at lower doses

- Total volume applied: 5 ml/kg
- Doses: 0, 10, 100 and 1000 mg/kg/day

SATELLITE GROUPS AND REASONS THEY WERE ADDED: 3 groups of 10M+10F treated and one group of 6M+6F controls for toxicokinetic studies after 26 weeks.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Twice daily
- Mortality: Twice daily
- Body weight: Weekly
- Food consumption: Weekly, food efficiencies calculated for first 14 weeks.
- Water consumption: Not recorded.
- Ophthalmoscopic examination: Prestudy and at weeks 12 and 25.
- Haematology: Samples obtained ex retro-orbital sinus from 10 rats/dose at weeks 12 and 25. Parameters monitored were Hb, PCV, RBC, WBC and differential count, platelet count, MCV, MCH, prothrombin time, abnormal cells, bone marrow smear.
- Biochemistry: Serum alkaline phosphatase, alanine and aspartate amino transferase, gamma-glutamyl transpeptidase, glucose, bilirubin, total cholesterol, urea, total triglyceride, total protein, Na, Cl, Ca, creatinine, inorganic phsohorus, electrophoretic protein.
- Urinalysis: From non-fasted water deprived rats. measurements were mde of pH, protein. Glucose, ketones, bilirubin, urobilinogen & blood (Multistiks), specific gravity, sediment analysis.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Full
- Organ weights: Adrenals, brain, kidneys, liver, lungs (with main stem bronchi), ovaries, pituitary , prostate, spleen, testes, thymus, thyroid, uterus (with cervix).
- Microscopic: adrenals, brain, eyes & optic nerve, femur, heart, kidneys, liver, lungs, seminal vesicles, spinal cord, stomach, thyroid, uterus.

OTHER EXAMINATIONS: Blood taken from satellite groups (3M+3F) non-fasted on days 1, during weeks 13 and 26 at 0,.5, 1, 2, 4, 8 and 24 hours after dosing.

STATISTICAL METHODS: Organ & body weights Bartletts test followed by either a Behrens Fischer test (if Bartletts

significant) or a Dunnetts test (if Bartletts not significant). Distribution of macroscopic and histopathological findings determined using a two-tailed Fischers Exact Test where appropriate. Haematological & biochemical parameters analysed using T-test.

Test substance: C22 alcohol - Docosanol (Behenyl alcohol)

Conclusion: NOAEL 1000 mg/kg/day. No adverse effects of statistical significance were seen in this well conducted study at any dose level. Cmax was reached in most instances at 1 hour post-dosing. Cmax and AUC increased with increasing dose level but the increase was not proportional.

Reliability: (2) valid with restrictions
Guideline study without detailed documentation (publication).

Flag: Critical study for SIDS endpoint

Reference: Iglesias, G, JJ Hlywka, JE Berg, MH Khalil, LE Pope and D Tamarkin. 2002a. The toxicity of behenyl alcohol: I. Genotoxicity and subchronic toxicity in rats and dogs. Regulatory Tox. and Pharm. 36, 69-79.

07-JAN-2006 (15)

<u>1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)</u>

Type: Sub-chronic
Species: dog **Sex:** male/female
Strain: Beagle
Route of administration: gavage
Exposure period: 26 weeks
Frequency of treatment: daily, 7 days/week
Post exposure period: no
Doses: 20, 200, 2000 mg/kg bw-day
Control Group: yes, concurrent vehicle
NOAEL: > 2000 mg/kg bw

Method: other: standard regulatory protocol
Year: 2000
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)

Result: NOAEL: 2000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0. 20, 200 and 2000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: No deaths among treated or control animals.

- Clinical signs: These were confined to observation of pale faeces in all dogs treated with 2000 mg/kg/day behenyl alcohol and 1 male and 3 females at 200 mg/kg/day. The incidence of this effect was variable and more pronounced in females. This was attributed to the presence in the gastrointestinal tract of unabsorbed test material. One control dog also had pale faeces on a single occasion.
- Body weight gain: No effects.
- Food/water consumption: No effects.
- Ophthalmoscopic examination: No treatment related changes.
- Clinical chemistry: No effects.
- Haematology: No effects.
- Urinalysis: No effects.
- Organ weights: No effects.
- Gross pathology: No adverse effects.
- Histopathology: No adverse effects.
- Other: Concentrations of behenyl alcohol in the blood were measured on day 1 and in weeks 13 and 26. Maximum mean plasma conc. (Cmax) was observed 2-16 hours after dosing independent of sex, dose level or sampling day. The rate and extent of systemic exposure to dogs as shown by AUC24 and Cmax on day 1 and in weeks 13 and 26 increased with increasing dose level. Increases were less than the proportionate dose increment and there was statistically significant evidence of non-proportionality on each sampling day.

STATISTICAL RESULTS: No statistically significant changes were observed in any of the parameters examined in the main study, the full results were therefore not presented in the publication. Statistical significance for reticulocytes, monocytes, basophils, eosinophils and large unstained cell counts was not reported as these data were not normally distributed.

Source: Iglesias, 2002a
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS
- Age: 19-23 weeks at start of study
- Number of animals: 4M+4F per dose level.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 26 weeks
- Type of exposure: Oral gavage
- Post exposure period: No
- Vehicle: 1% aqueous Tween 80
- Concentration in vehicle: 20% diluted to give standard volume.
- Total volume applied: 10 ml/kg

- Doses: 0, 20, 200 and 2000 mg/kg/day

SATELLITE GROUPS AND REASONS THEY WERE ADDED: None

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Twice daily, full vetinary examination prestudy & weeks 11 & 24.
- Mortality: Daily
- Body weight: Weekly
- Food consumption: Weekly, food efficiency calculated weekly up to week 14.
- Water consumption: not recorded
- Ophthalmoscopic examination: Prestudy and weeks 12 & 25.
- Haematology: All dogs ex jugular vein, prestudy & weeks 12 & 25. Hb, PCV, RBC, WBC with differential count, platelets, MCV, MCH, prothrombin time, activated partial thromboplastin time, bone marrow samples taken from iliac crest at study end.
- Biochemistry: All dogs, prestudy & weeks 12 & 25. Serum alkaline phosphatase, alanine and aspartate amino transferase, gamma-glutamyl tracspeptidase, glucose, bilirubin, total cholesterol and trigyceride, total protein, Na, K, Cl and Ca. Inorganic phosphorus, electrophoretic protein, creatinine phosphokinase.
- Urinalysis: Fasted animals weeks 12 & 25. pH, protein. Glucose, ketones, bilirubin, urobilinogen & blood (Multistiks), specific gravity, ntirites & total reducing substances, sediment analysis.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Full
- Organ weights: Adrenals, brain, kidneys, liver, lungs, ovaries, pituitary, prostate with urethra, spleen, testes, thymus, thyroid, uterus (with cervix).
- Microscopic: adrenals, brain, eyes & optic nerve, heart, kidneys, liver, lungs, spinal cord, stomach, thyroid, uterus.

OTHER EXAMINATIONS: Blood samples taken from all rats prestudy and during weeks 13 & 26 at 0.5, 1, 2, 4, 8 and 24 hours after dosing for toxicokinetic studies.

STATISTICAL METHODS: Organ & body weights Bartletts test followed by either a Behrens Fischer test (if Bartletts significant) or a Dunnets test (if Bartletts not significant). Distribution of macroscopic and histopathological findings determined using a two-tailed Fischers Exact Test where appropriate. Haematological & biochemical parameters and

urinalysis was analysed using T-test.

Test substance: C22 alcohol - Docosanol [661-19-8] (Behenyl alcohol)

Conclusion: NOAEL 2000 mg/kg/day (dogs). No adverse effects were seen in this well conducted study at any dose level. Cmax was reached at 2-16 hours post-dosing. Cmax and AUC increased with increasing dose level but the increase was not proportional.

Reliability: (2) valid with restrictions
Guideline study without detailed documentation (publication).

Reference: Iglesias, G, JJ Hlywka, JE Berg, MH Khalil, LE Pope and D Tamarkin. 2002a. The toxicity of behenyl alcohol: I. Genotoxicity and subchronic toxicity in rats and dogs. Regulatory Tox. and Pharm. 36, 69-79.

06-AUG-2005 (15)

1-Tetracosanol, 1-Hexacosanol, 1-Octacosanol, and 1-Triacontanol for their respective Aluminum Salts

Species	:	dog
Sex	:	male/female
Strain	:	Beagle
Route of admin.	:	gavage
Exposure period	:	1 year
Frequency of treatment	:	daily, 7 days/week
Post obs. period	:	none
Doses	:	50, 250 mg/kg bw
Control group	:	yes
NOAEL	:	= 250 mg/kg bw
Method	:	other
Year	:	2001
GLP	:	no data
Test substance	:	C24-34 alcohols
Test substance	:	C24-34 even chain alcohols (D-002) primarily isolated and purified from beeswax, composition as follows: triacontanol 26.63% octacosanol 17.49% dotriacontanol 16.95% hexacosanol 15.34% tetracosanol 13.24% tetratriacontanol % 2.23% Other well-known, nonactive components 7.12%
Test condition	:	TEST ORGANISMS - Age: 10-12 weeks

- Weight at study initiation: 8-12 kg
- Number of animals: 4M+4F per group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 1 year
- Type of exposure: oral gavage
- Post exposure period: none
- Vehicle: 1% acacia gum in water
- Concentration in vehicle: Varied according to dose level.
- Total volume applied: 8 ml/kg
- Doses: 0, 50, 250 mg/kg/day (250 mg/kg/day was the highest level which could be given in a single dose because of solubility considerations)

SATELLITE GROUPS AND REASONS THEY WERE ADDED:

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily
- Mortality: Daily
- Body weight: Monthly
- Food consumption: Daily
- Water consumption: Not recorded
- Ophthalmoscopic examination: None
- Haematology: Venous blood prestudy and at 3 monthly intervals. Hb & heamatocrit only were determined.
- Biochemistry: Venous blood prestudy and at 3 monthly intervals. glucose, aspartate and alanine transferases, creatinine and acetyl cholinesterase.
- Urinalysis: Not done.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Full necropsy.
- Organ weights: Liver, kidneys, heart, lungs, spleen, thymus, adrenals, testis, prostate (not ovaries)
- Microscopic: All major organs including gonads.

STATISTICAL METHODS: Body weight, organ weight and blood parameters were analysed with a variance analysis (Kruskall-Wallis non-parametric ANOVA test). Histopathological results were compared using Fischers exact test. $P<0.05$ was established for statistical significance.

Result : NOAEL (NOEL): 250 mg/kg/day (highest dose level tested)

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX 0, 50 and

250 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: None
- Clinical signs: None
- Body weight gain: No significant differences between treated and control groups.
- Food consumption: Not reported.
- Clinical chemistry: No significant differences.
- Haematology: No significant differences.
- Organ weights: No significant differences.
- Gross pathology: Normal
- Histopathology: No treatment related changes. Autoimmune thyroiditis was observed in one control female. 1 treated male dog at each dose level also showed this type of lesion associated with adenitis. Particular attention was paid to examination of the stomach as a target organ for anti-ulcer drug toxicity (D-002 is used as an anti-ulcer drug). There was no evidence of any damage to the gastric mucosa.

Conclusion : NOAEL 250 mg/kg/day (highest dose level tested). No treatment related adverse effects were observed in this study which included histopathological examination of the male and female reproductive organs.

Reliability : (2) valid with restrictions
Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment.

Source : Aleman 2001.
Hayes Consultancy Service Bromley, Kent

Reference Aleman, C., Rodeiro, I., Noa, M., Menendez, R., Gamez, R., Hernandez, C., and Mas, R. 2001. One-year dog toxicity study of D-002, a mixture of aliphatic alcohols. J. Appl. Toxicol. 21:179-184.

24.01.2005 (1)

<u>1-Tetracosanol, 1-Hexacosanol, 1-Octacosanol, and 1-Triacontanol for their respective Aluminum Salts</u>

Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : gavage
Exposure period : 14 days

Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	2000, 3000, 5000 mg/kg/day
Control group	:	no data specified
NOAEL	:	> 5000 mg/kg bw
Method	:	other: screening
Year	:	1998
GLP	:	no data
Test substance	:	C24-C34 alcohols
Test substance	:	C24-34 even chain alcohols (D-002) primarily isolated and purified from beeswax, composition as follows: triacontanol 26.63% octacosanol 17.49% dotriacontanol 16.95% hexacosanol 15.34% tetracosanol 13.24% tetratriacontanol % 2.23% Other well-known, nonactive components 7.12%
Test condition	:	The test material D-002 was prepared as a suspension in acicia gum/water (10 mg/ml). Groups of 5M+5F rats reeceived daily doses of 2000, 3000 or 5000 mg/kg for 14 dyas. Clinicals signs were observed regualrly and body weights recorded prior to the first treatment then at 7 and 14 days. Biochemical determinations and histopathological examination was carried out at the end of the study.
Result	:	There were no adverse effects on any of th eparameters studied. The 14 day LD50 was >5000 mg/kg.
Reliability	:	(2) valid with restrictions
Reference		Rodeiro, I. et al, 1998 Preclinical oral toxicology in rats of D-002, a natural drug with antiulcer effects. Drug Chem. Tox. 21(2): 151-162.
16.05.2005		(7)

<u>1-Tetracosanol, 1-Hexacosanol, 1-Octacosanol, and 1-Triacontanol for their respective Aluminum Salts</u>

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	90 days

Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	0, 5, 25, 125, 625 mg/kg/day
Control group	:	yes
NOAEL	:	> 625 mg/kg bw
Method	:	other:
Year	:	1998
GLP	:	no data
Test substance	:	C24-34 alcohols

Test substance : C24-34 even chain alcohols (D-002) primarily isolated and purified from beeswax, composition as follows:

triacontanol 26.63%
octacosanol 17.49%
dotriacontanol 16.95%
hexacosanol 15.34%
tetracosanol 13.24%
tetratriacontanol % 2.23%
Other well-known, nonactive components 7.12%

Test condition : TEST ORGANISMS SD rats
- Age: 6-8 weeks
- Weight at study initiation: 150-200 g
- Number of animals: 12M+12F/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 90 days
- Type of exposure: gavage
- Post exposure period: none
- Vehicle: As a suspenson in acacia gum/water
- Concentration in vehicle: 10 mg/ml
- Doses: 0, 5, 25, 125, 625 mg/kg/day

SATELLITE GROUPS AND REASONS THEY WERE ADDED:
None

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily
- Mortality: Daily
- Body weight: Weekly
- Food consumption: Weekly
- Water consumption: Not recorded
- Ophthalmoscopic examination: No data
- Haematology: Haemoglobin, Haematocrit, total and differential

white cell count.
- Biochemistry: At the end of the assay. ALAT, ASAT, creatininte, acetyl cholinesterase, alkaline phosphatases, creatin-kinase, urea.
- Urinalysis: No

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Organ weights are reported for liver, kidney, Heart, Lungs, Spleen and Thymus, organs examined as described for NTP studies, 1990.
- Microscopic: Tissues examined as described for NTP studies, 1990. (Chhabra et al, NTP program, 1990)

STATISTICAL METHODS: ANOVA for body weight, food consumption, blood parameters and organ weights. Fischers Exact test for mortality, clinical observations and histopathological findings.

Result : NOAEL: >625 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX 5, 25, 125, 625 mg/kg/day
- Time of death: No data
- Number of deaths at each dose: 1M control, 1M+1F at 5 mg/kg, 2M+1F at 625 mg/kg, confirmed by autopsy as due to the gavage procedure.

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Clinical signs: Similar in treated and control animals.
- Body weight gain: Similar in treated and control animals.
- Food consumption: Similar in treated and control animals.
- Clinical chemistry: Similar in treated and control animals.
- Haematology: Similar in treated and control animals.
- Organ weights: Similar in treated and control animals.
- Gross pathology: Similar in treated and control animals.
- Histopathology: Similar in treated and control animals and in comparision with historical controls.

STATISTICAL RESULTS: No changes of statistical significance.

Conclusion : The NOAEL for this rat 90 day gavage study was >625 mg/kg/day. There were no treatment related changes in any of the parameters tested.

Reliability : (2) valid with restrictions
Study well documented, meets generally accepted scientific

principles, acceptable for assessment. Although not reported as being carried out to any specific regulatory guideline the conduct of the study appeared to similar to that required for a guideline study and the publication provided a good level of detail.

Flag : Critical study for SIDS endpoint

Reference Rodeiro, I. et al, 1998 Preclinical oral toxicology in rats of D-002, a natural drug with antiulcer effects. Drug Chem. Tox. 21 (2): 151-162.

16.05.2005 (7)

1-Tetracosanol, 1-Hexacosanol, 1-Octacosanol, and 1-Triacontanol for their respective Aluminum Salts

Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : gavage
Exposure period : 1 year
Frequency of treatment : daily
Post obs. period : none
Doses : 0, 250, 500 and 1000 mg/kg
Control group : yes
NOAEL : > 1000 mg/kg bw
Method : other:
Year : 1998
GLP : no data
Test substance : C24-34 alcohols

Test substance : C24-34 even chain alcohols (D-002) primarily isolated and purified from beeswax, composition as follows:

triacontanol 26.63%
octacosanol 17.49%
dotriacontanol 16.95%
hexacosanol 15.34%
tetracosanol 13.24%
tetratriacontanol % 2.23%
Other well-known, nonactive components 7.12%

Test condition : TEST ORGANISMS SD rats
- Age: 6-8 weeks
- Weight at study initiation: 150-200 g
- Number of animals: 20M+20F/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 1 year

- Type of exposure: gavage
- Post exposure period: none
- Vehicle: As a suspenson in acacia gum/water
- Concentration in vehicle: 10 mg/ml
- Doses: 0, 250, 500 and 1000 mg/kg

SATELLITE GROUPS AND REASONS THEY WERE ADDED: None

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily
- Mortality: Daily
- Body weight: Weekly
- Food consumption: Weekly
- Water consumption: Not recorded
- Ophthalmoscopic examination: No data
- Haematology: Haemoglobin, Haematocrit, total and differential white cell count.
- Biochemistry: At the end of the assay. ALAT, ASAT, creatininte, acetyl cholinesterase, alkaline phosphatases, creatin-kinase, urea.
- Urinalysis: No

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Organ weights are reported for liver, kidney, Heart, Lungs, Spleen and Thymus, organs examined as described for NTP studies, 1990.
- Microscopic: Tissues examined as described for NTP studies, 1990. (Chhabra et al, NTP program, 1990)

STATISTICAL METHODS: ANOVA for body weight, food consumption, blood parameters and organ weights. Fischers Exact test for mortality, clinical observations and histopathological findings.

Result : NOAEL: >1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX 5, 25, 125, 625 mg/kg/day
- Time of death: No data
- Number of deaths at each dose: 1M+1F control, 2M+1F at 250 mg/kg, 2M+2F at 500 and 1000 mg/kg, confirmed by autopsy as due to the gavage procedure.

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Clinical signs: Similar in treated and control animals.
- Body weight gain: Similar in treated and control animals. However

a slight non-significant decrease in bodyweight gain was observed at the top dose level.
- Food consumption: Similar in treated and control animals.
- Clinical chemistry: Similar in treated and control animals.
- Haematology: Similar in treated and control animals.
- Organ weights: Similar in treated and control animals.
- Gross pathology: Similar in treated and control animals.
- Histopathology: Similar in treated and control animals and in comparision with historical controls.

STATISTICAL RESULTS: No changes of statistical significance.

Conclusion : Rat gavage study NOAEL 1000 mg/kg/day for 1 year. A slight decrease in bodyweight gain in top dose animals was not of statistical significance. All other endpoints showed no adverse effect.

Reliability : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment. Although not reported as being carried out to any specific regulatory guideline the conduct of the study appeared to similar to that required for a guideline study and the publication provided a good level of detail although not at the individual animal level.

Flag : Critical study for SIDS endpoint

Reference Rodeiro, I. et al, 1998 Preclinical oral toxicology in rats of D-002, a natural drug with antiulcer effects. Drug Chem. Tox. 21(2):151-162.

16.05.2005 (7)

5.5 Genetic Toxicity 'in Vitro' (Bacterial Test)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type Ames test
System of testing TA97, 98, 100, 104 and 1535
Test concentration 1, 3, 10, 33, 100, 333, 1,000, 3,333, 10,000 microgram/plate
Cycotoxic concentr. Not determined
Metabolic activation with and without
Result Negative
Method Other

Year 1992
GLP no data
Test substance other TS: 91 % pure ethanol (64-17-5)

Method No. of replicates: 5 + complete repeat of experiment. Frequency of dosing: Once, including pre-incubation.

	Positive and negative controls: Positive controls were included. No. of meta phases analyzed: Not applicable. Solvent used: Not applicable. Follow-up: Not applicable. Criteria for evaluating results: Combination of magnitude of increase in number of his+ revertants and shape of dose-response curve. Positive controls (-S9): sodium azide (for TA1535, TA100), 9-aminoacridine (TA97), 4-nitro-o-phenylenediamine (TA98), methylmethane sulphonate (TA104). Positive control (+S9): 2-aminoanthracene. Solvent control: water.
Remark	A preincubation assay. This test is considered to be highly reliable in view of inclusion in NTP mutagenicity testing program, conducted in 5 strains over a wide range of concentrations, with and without two metabilic induction systems in two concentrations.
Result	Negative.
Conclusion	Test-specific confounding factors: None. Dose-effected related observations: Ethanol at any dose did not produce a 2-fold increase in his+ revertants in the absence or presence of rat or hamster liver extracts. Mitotic index: Not applicable. Ethanol failed to induce reversions in any S. typhimurium tester strain with or without metabolic activation over a wide range of doses up to 10 mg/plate.
Reliability	(1) valid without restriction
Flag	Critical study for SIDS endpoint
Reference	Zeiger, E., Anderson, S., Haworth, S., Lawlor, T, Mortelamns, K. (1992). Salmonella mutagencity tests: V. Results from the testing of 311 chemicals. Environ Mol Mut 19; 2-141.
12.11.2004	(218)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Ames test
System of testing	Salmonella typhimurium/microsome test
Test concentration	100 microlitre
Cycotoxic concentr.	Not determined
Metabolic activation	with and without
Result	Negative
Method	Other
Year	1982
GLP	no data

Test substance	ethanol (64-17-5)
Method	Test design: Salmonella/microsomal assays were carried out by making post-mitochondrial preparations from livers of male Sprague-Dawley rats induced with Aroclor 1254. Reversion of all strains by 5 microgram/plate of the promutagen 2-aminoanthracene was included in each assay system. Ethanol was one of 25 chemicals examined by spot testing with 5 microgram with and without 89 mix. Compounds positive in the spot test were then subject to plate incorporation testing (not necessary for ethanol). Ethanol was actually being used as an inert solvent. Positive and negative controls: Both negative controls and positive (2-aminoanthracene, 4-nitro-o-phenylene diamine [frameshift mutagen, 9-aminoacridine [frameshift mutagen and sodium azide [base-pair substitutions]) were used. The Salmonella histidine auxotrophs hisTA98, hisTA100, hisTA1535, hisTA1537 and hisTA1538 were used.
Result	No evidence of mutagencity was observed for ethanol with and without 59 mix. 9 of 25 chemicals demonstrated potential mutagenicity in the spot test but only one of these, DEA laureth sulphate, gave a positive test in the plate incorporation test.
Reliability	(2) valid with restrictions Spot testing with confirmatory incorporation testing with 4 positive controls indicates a valid study. However, there is no mention of Good Laboratory Practice.
Reference	Blevins, R.D., Taylor, D.E. (1982). Mutagencity screening of twenty five cosmetic ingredients with the Salmonella microsome test. J Environ Sci Health 1982; A17 (2): 217-239.
12.11.2004	(219)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Ames test
System of testing	Salmonella/microsome
Test concentration	10, 100,500, 1000 microgram/plate
Cycotoxic concentr.	
Metabolic activation	With
Result	Negative
Method	Other
Year	1975
GLP	no data

Test substance	95 – 99.9% ethanol (64-17-5)
Method	Ethanol was one of 300 chemicals tested in the standard Salmonella/microsome Ames test using human or rat liver S9 mix. The test method is given in detail in Ames, McCann and Yamasaki (1975) Mutat Res. and is reviewed in McCann & Ames (1975) Ann N.Y. Acad Scl. Salmonella typhimurium strains TA1535, TA1537, TA100 and TA9S were used.
Remark	It is noted that there was a high correlation between carcinogenicity and mutagenicity (90%; 156 carcinogens in 174 mutagens) whereas few noncarcinogens showed any degree of mutagenicity.
Result	There were < 70 revertants per 10,000.
Reliability	(1) valid without restriction The methodology of this test is now accepted and repeatedly used as a standard in vitro test for mutagenicity. It is considered robust for detecting environmental carcinogens. This study is regarded as valid without restrictions.
Reference	McCann, J., Choi, E., Yamasaki, E., Ames, B.N. (1975) Detection of carcinogens as mutagens in the Salmonella/microsome terst: Assay of 300 chemicals. Proc Nat Acad Sd 1975; 72 (12): 5135-5139.
12.11.2004	(220)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Ames test
System of testing	Salmonella typhimurium L T2 strains
Test concentration	100 microlitre
Cycotoxic concentr.	not presented
Metabolic activation	with and without
Result	Negative
Method	Other
Year	1983
GLP	no data
Test substance	ethanol (64-17-5)
Method	Different concentrations of 9 delta-tetrahydrocannabinol and positive mutagen controls were added in 0.1 ml proportions together with 0.1 ml of a 16 hr nutrient broth culture of the bacterial test strain or 0.1 ml of the culture and 0.5 ml of $-9 mix. These were then poured onto minimal glucose agar plates to form an even layer across the agar.

	Duplicate plates were made for each strain and plates were incubated for 48 hr at 37 degC. Colonies were counted on a Quebec colony counter. Background lawn and unreverted bacteria were evaluated by microscopy. Appropriate control combinations and growth study plates were prepared.
Remark	Salmonella typhimurium strains TA1538, TA1537, TA1535. TA100 and TA98. This study incorporated ethanol as a negative control in an evaluation of the mutagenicity of delta9-tetrahydrocannabinol and other mutagens. Absolute ethanol was used as the solvent for 9-aminoacridine, one of the positive mutagen controls.
Result	No evidence of mutagencity was observed in the absence or presence of S9mix.
Reliability	(2) valid with restrictions The study gave the results expected for positive controls and ethanol evaluated as a solvent to a positive control gave negative results with and without S-9 mix. However, there is no mention of Good Laboratory Practice.
Reference	Blevins, RD., Shelton, M.S. (1983). Response of Salmonella typhimurium mutants to delta-9-THC and in conjunction with known mutagens. J Environ Sci Health A18 (3), 413-443.
12.11.2004	(221)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	other: Ames reversion test and DNA repair test in E. coli
System of testing	Salmonella typhimurium strains
Test concentration	TA98, TA100, TA1535, TA1537, TA1538 and E.coli strains
Cycotoxic concentr.	Tested to "toxicity limit" (not defined).
Metabolic activation	with and without
Result	Ambiguous
Method	Other
Year	1984
GLP	no data
Test substance	ethanol (64-17-5)
Method	Ethanol tested in revised plate incorporation test as described in Maron, D.M. & Ames, B.N. (1983) Revised methods for the Salmonella mutagenicity test, Mutation Res.113; 173-215. The Ames reversion test was conducted with his- S. typhirnuriurn strains TA1535, TA1537, TA1538, TA98, TA100 and, in part,

	TA97. 89 Mix contained 10% liver S9 fractions from Sprague-Dawley rats pretreated with Aroclor 1254. Mutagenic potency was expressed by dividing the number of revertants in excess of controls by the corresponding amount of ethanol in nrnoles. The genotoxic activity of Escherichia coli was assessed using strains WP2 (repair proficient), WP67 and CM871. A ratio of more than 2 between the MIC's in repair proficient (rep+) anddeficient (rep-) strains was considered to be sufficient.
Result	All strains of Salmonella typhirnurium showed no reversion in the presence of ethanol with potency (revertants/nmole of <0.00006. I n the DNA repair test there was equivocal activity in the 2 hr preincubation assay in the presence of S9, otherwise, ethanol was inactive in the absence of S9 and in the spot test.
Test Substance	Reagent grade
Reliability	(2) valid with restrictions Consistency of results in the two tests for 71 % of the substances tested together with an overall predictive accuracy of 64.5% for the reversion test and 72.4% for the DNA-repair test in 75 compounds classified for their carcinogenic activity, demonstrated the validity of this study on comparability of methods. This study is considered to be valid with restrictions.
Reference	De Flora, S., Zanacchi, P., Camoirano, A., Bennicelli, C, Badolati. G.S. (1984). Genotoxic activity and potency of 135 compounds in the Ames reversion test and ina bacterial DNA repair test. Mutation Res.133; 161-198.
12.11.2004	(222)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Ames test
System of testing	Salmonella typhimurium strains TA97 and TA102
Test concentration	
Cycotoxic concentr.	
Metabolic activation	with and without
Result	negative
Method	
Year	1984
GLP	no data

Test substance	95 – 99.9% ethanol (64-17-5)
Method	Plate incorporation test (as described in Maron and Ames - 1983. Muta Res 113, 173.) S9 mix contained 10% liver S9 from SD rats pretreated with Aroclor 1254. Mutagenic potential expressed by dividing number of revertants in excess of controls by corresponding amount of compound in nmoles.
Result	Ethanol was negative for mutagenic activity in the Ames reversion test using strain T A9? but showed a reproducible increase in revertants over controls in TA102 but this was less than two-fold increase which is not normally considered to be biologically significant in the Ames test. It was however repeatable. The authors tentatively classified it as an uncertain or questionable mutagen. However, considering the response against the high dose used (160mg/plate) sU\:igests< that this is an excessively conservative conclusion and that the balance of evidence points to a negative result. Source from Carlo Erba
Reliability	(2) valid with restrictions
Reference	De Flora, S., Camoirano, A., Zanacchi, P., Bennicelli, C. (1984). Mutagenicity testing with TAg? and TA102 of 30 DNA-damaging compounds negative with other Salmonella strains. Mutat Res 134:159-165.
12.11.2004	(223)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Ames test
Metabolic activation	with and without
Year	1997
GLP	yes
Test substance	ethanol (64-17-5)
Remark	Ethanol has been reported as being compatible with the Salmonella/microsome test at 200ullplate in the plate incorporation assay and up to 100 µl/plate in the pre-incubation assay (Maron et al., 1981). At Safepharm Laboratories, ethanol has been used as one of the validated vehicle controls for more than 10 years. The typical dose volume used is 100 µl/plate, which is equivalent to 79 mg/plate, or approximately 16 times the normal maximum recommended dose level of 5 mg/plate used in regulatory mutagenicity tests. In 1998 it was used as the vehicle for 18 test materials, which was approximately 5% of the total number of

	studies completed in that year. The mean, minimum and maximum frequencies of revertant colonies for the ethanol vehicle control plates were all comparable to the 1998 vehicle control history profile for all vehicle controls used at Safepharm Laboratories in 1998.
Reliability	(2) valid with restrictions
Reference	Phillips P. J., Jenkinson, P. (2001) Is ethanol genotoxic? A review of the published data. Mutagenisis 16, 2, 91-101.
29.06.2004	(20)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	DNA damage and repair assay
System of testing	343/636 (genotype uvrB+/recA+/lac-) and DNA repair deficient 343/591 (uvrB-/recA-/lac+)
Test concentration	Up to 1720 mmol/l
Cycotoxic concentr.	>1720 mmol/l
Metabolic activation	with and without
Result	negative
Method	other
Year	1992
GLP	no data
Test substance	ethanol (64-17-5)
Method	Differential DNA repair test as described by Mohn, G.R. et al. (1984) Methodologies for the direct and animal mediated determination of various genetic effects in derivatives of strain 343/113 of E. coli K-12, in: B.J. Kilbeyet al. (Eds.) Handbook of Mutagenicity Test Procedures, 2nd OOn., Elsevier, Amsterdam, pp. 189 - 215. For each concentration of test compound 100 ul of test compound or the solvent, 100 ul of bacterial mix and 500 ul S9 mix (where used) were made up to 1 ml with buffered saline. The mixture was incubated at 37 degG in the dark before seeding NR agar plates. The relative survival of DNA repair deficient and proficient bacteria were calculated. Solvent not specified, but since ethanol was a solvent used for other compounds and a high concentration was used, it is likely no solvent was used. Controls: The positive control was 4~nitroquinoline-N-oxide without S9 mix. No positive control was used for the S9. mix as this had been

	previously validated. Statistical methods: confidence interval determined according to the variance of each strain, determined from an experiment with 100 untreated samples. A reduction in number of colonies by 2 standard deviations taken as significant.
Remark	This study was a screening test of 61 compounds, giving a mixture of positive and negative results.
Result	In both the absence and presence of S9 mix, the high dose of 1720 mmole/l ethanol gave a negative result in DNA repair deficient strain of E. coli. Test substance was of the highest purity obtainable from commercial sources. (2) valid with restrictions
Reliability	Although conducted to a standard published method this paper does not present method detail in full. There was an overall concordance of 80%> between this and the results from Ames tests on the 51 chemicals studied. The study is therefore considered to be valid with restrictions.
Reference	Hellmer, L. and Bolcsfoldi, G. (1992) An evaluation of the E. coli K-12 uvrBlrecA DNA repair host-mediated assay. Mutation Res. 272;145-160.
12.11.2004	(224)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Bacterial forward mutation assay
System of testing	Escherichia coli RK+ (replicative killing competent strain CHY832)
Test concentration	11 to 23% v/v
Cycotoxic concentr.	17% v/v
Metabolic activation	without
Result	positive
Method	other
Year	1985
GLP	no data
Test substance	ethanol (64-17-5)
Method	Test design: The test strain carries a lethal gene (RK+) that is repressed below 39 degC and derepressed above this temperature. After treatment with ethanol at 30 degC cells were plated and cultured at 42 degC to detect RK- mutants. No. of replicates: 3 per concentration. Frequency of dosing: exposure to ethanol for 10 min before

	plating. Positive and negative controls: Negative controls were used. No. of meta phases analyzed: Not relevant. Solvent: with and without DMSO. Evaluation criteria: Positive result when mutation index twice that of control.
Remark	The authors suggest that there is a threshold concentration below which ethanol is not genotoxic. This concentration appears to be the upper limit for cellular tolerance to ethanol. Whilst positive, the massive concentration at which this result was seen can be extrapolated to conclude that the result would be negative at more conventional test concentrations.
Result	The 5 ethanol preparations showed similar dose-response curves for induction of RK- mutants with thresholds of 18-19% v/v. Addition of dimethylsulfoxide lowered the thresholds by around 5% to 13-15%. Test-specific confounding factors: None. Dose-effect related observations: All ethanol preparations induced RKmutants with mutation indices of 2 or more. Steep dose-reponse curves showed threshold at 18-19% v/v. Frequency of reversions etc: All preparations gave mutation indices of up to 50 at the highest dose tested. ; Mitotic idex: Not relevant.
Test Substance	Synthetic anhydrous 100%, synthetic 95%, 95% grain alcohol, 96.6% grain alcohol and dehydrated absolute 100% grain alcohol. The positive result could be due to trace contaminants in ethanol, a bacterial metabolite, direct mutagenic effect of ethanol and indirect effect of ethanol.
Reliability	(2) valid with restrictions
Reference	Hayes, S. (1985). Ethanol-induced genotoxicity. Mutat. Res. 143: 23-27.
12.11.2004	(225)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Bacterial reverse mutation assay
System of testing	Escherichia coli
Test concentration	140 or 180 mg/ml
Cycotoxic concentr.	
Metabolic activation	with and without
Result	positive
Method	other

Year	1984
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	The escherichia coli selector strain CHY832 deleted for bio-uvr-chIA was used with and without 89 activation to examine the mutagenic potential of 48 environmental chemicals including ethanol. The study was run parallel with the McCann and Ames Mutatest.
Remark	In the Mutatest, ethanol was negative for mutagenicity at 10000 microg/ml with S9. In the RK test, ethanol was positive for mutagenicity at 180000 microg/ml without S9
Reliability	(4) not assignable
Reference	Hayes, S., Gordon, A., Sadowski, I., Hayes, C. (1984). RK bacterial test for independently measuring chemical toxicity and mutagenicity: Short-term forward selection assay. Mutat Res 130: 97-106.
12.11.2004	(226)

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Test substance:	1-Butanol, from Mallinkrodt
Test species/strain:	Salmonella typhimurium: Strains, TA98, TAIOO, TA1535, TAl537
Test method:	Standard Salmonella plate incorporation test, with and without PCB-induced rat liver S9 metabolic activation.
GLP:	No
Test results:	Minimum concentration of test substance at which toxicity to bacteria was observed: with metabolic activation: >10 µg/plate without metabolic activation > 10 µg/plate Concentration oftest compound resulting in precipitation:
Number of revertants:	< 0.0005 revertants/nmole, < 70 revertants/10^4 µg/plate

Genotoxic effects:

	+	?	-
with metabolic activation:	[ ]	[ ]	[X]
without metabolic activation:	[ ]	[ ]	[X]

Comments: No evidence of mutagenic activity in reverse point mutation assay in Salmonella with or without a metabolic activation system from

arochlor treated rat liver homogenate.
The mice were sacrificed 24 and 48 hours postdosing and evaluated for clastogenicity and spindle poison effects. Positive and negative controls all produced appropriate responses. BA did not produce any chromosome-damaging (c1astogenic) effect, and there were no indications of any impairment of chromosome distribution in the course of mitosis (spindle poison effect).

References: The Salmonella typhimurium/mammalian microsomal assay, a report of the U.S. EPA Gene-Tox Program, Kier, L.E., et al. Mutation Research 168(2):69-240. 1986.

McCann J., Choi E., Yamasaki E. andArnes B.N. (1975) Detection of carcinogens as mutagens in the Salmonella/ microsome test: Assay of 300 chemicals. Proc. Nat. Acad. Sci. 72: 5135-5139.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: other: Bacterial reverse mutation assay (Ames Test)
System of testing: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
Concentration: 1st test: 8,40, 200, 1000 and 5000 ug/plate 2nd test: 6.25, 25, 100, 400 and 1600 ug/plate
Cytotoxic Concentration: 5000 ug/plate
Metabolic activation: with and without
Result: negative

Method: OECD Guide-line 471
Year: 1990
GLP: yes
Test substance: >95% 1-hexanol (111-27-3)

Result: GENOTOXIC EFFECTS:
- With and without metabolic activation: No significant increase above control levels in either series of tests.

PRECIPITATION CONCENTRATION: No precipitation.

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: complete or partial inhibition of background lawn observed in all strains at 5000 ug/plate (except TA 100 where no inhibiton was observed)

TEST-SPECIFIC CONFOUNDING FACTORS: None
Source: Henkel 1990
Hayes Consultancy Service Bromley, Kent

Test condition: METHOD

Bacterial reverse mutation assay OECD 471. 2-aminoanthracene was the only indicator of S9 efficacy, however all the cultures treated with 2-AA in the presence of S9, showed a clear increase in reverse mutation rate compared to controls. The activity of the S9 was confirmed against strain TA98 using 2AA and benzo[a]pyrene. A cytogenetic test with cyclophosphamide was also carried out.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium stains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced. The activity of the S9 was confirmed against strain TA98 using 2AA and benzo[a]pyrene. A cytogenetic test with cyclophosphamide was also carried out.

ADMINISTRATION:
- Dosing: 1st test: 8,40, 200, 1000 and 5000 ug/plate
2nd test: 6.25, 25, 100, 400 and 1600 ug/plate suspended in Tween 80/aqueous.
- Number of replicates: three
- Application: Plate incorporation
- Positive and negative control groups and treatment: Positive controls were 2-amino anthracene 5 ug/plate all strains; sodium azide 2 ug/plate; 9-amino acridine (80 ug/plate; 4-nitro-o-phenylene diamine 40 ug/plate. Negative controls Tween 80/aqueous and untreated fresh cell suspensions in buffer.
- Incubation: 48 hours at 37C

CRITERIA FOR EVALUATING RESULTS: Combination of: a) Plate background of non-reverted bacteria not showing growth reduction vs respective negative controls. b) Spontaneous mutation rates within historical limits. c) At one or more doses tested the substance causes a 2 (TA 100) or 3 (other strains) fold increase in mutation rate above control levels.

Test substance: Tradename Lorol C6 (98% pure)

Conclusion: The C6 alcohol Lorol C6 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 5000 ug/plate (cytotoxicity observed at 5000 ug/plate).
Reported in Iuclid 2000.

Reliability: (1) valid without restriction

Guideline study.
Flag: Critical study for SIDS endpoint
Reference: Henkel KGaA. 1990. Report Lorol C6 98% salmonella/mammalian-microsome mutagenicity test (Ames test). Unpublished data, Report No. TDB 900320.

Iuclid 2000 European Commission - European Chemicals Bureau
hexan-1-ol Cas# 111-27-3
11-NOV-2004 (25) (29)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Type: other: Bacterial reverse mutation assay (Ames Test)
System of testing: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
Concentration: 4, 20, 100, 500, and 2500 ug/plate
Cytotoxic Concentration: 2500 ug/plate for all strains, 500 ug/plate for some strains (see text)
Metabolic activation: with and without
Result: negative

Method: other: An in-house protocol similar to OECD No. 471
Year: 1982
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Result: GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain tested. Positive controls showed an appropriate increase in reverse mutation rate.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION:
- With metabolic activation: Total inhibition of bacterial growth at 2500 ug/plate for all strains tested also at 500 ug/plate for strains TA1537, 1538 and 98.
- Without metabolic activation: Total inhibition of bacterial growth at 2500 ug/plate for all strains tested also at 500 ug/plate for strains TA1538 and 98.

Source: Henkel KGaA 1982a
Hayes Consultancy Service Bromley, Kent
Test condition: METHOD Bacterial reverse mutation assay based on OECD 471. Full experimental details were not provided but actual results were available. 2-aminoanthracene was the only indicator of efficacy of the S9 mix however there was a clear increase in

reverse mutation rate in bacteria treated with 2-AA in the presence of S9 compared to controls.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 0, 4, 20, 100, 500, and 2500 ug/plate suspended in Tween 80/aqueous
- Number of replicates: Four per dose level.
- Application: Plate incorporation.
- Positive and negative control groups and treatment: Positive controls were 2-amino anthracene 5 ug/plate, sodium azide 1 ug/plate; 4-nitro-o-phenylene diamine 40 ug/plate.

CRITERIA FOR EVALUATING RESULTS: Not specifically reported assume as OECD 471.

Test substance: Tradename Lorol C8

Conclusion: The C8 alcohol Lorol C8 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 2500 ug/plate. Cytotoxicity was observed at the highest dose level tested.

Cited in Iuclid 2000.

Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions (limited reporting).

Flag: Critical study for SIDS endpoint

Reference: Henkel KGaA. 1982a. 1-Octanol: Evaluation of mutagenicity. Unpublished data, Report No. TBD 820114. Publication no. 294.

Iuclid 2000 European Commission - European Chemicals Bureau
Octan-1-ol Cas# 111-87-5
16-JUL-2005 (51) (62)

<u>1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)</u>

Type: other: Bacterial reverse mutation assay (Ames test)

System of testing: Salmonella typhimurium strains TA98 and TA100

Concentration: 50, 158, 500, 1580, 5000 ug/plate

Cytotoxic Concentration: No cytotoxicity observed.
Metabolic activation: with and without
Result: negative

Method: other: Ames
Year: 1996
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Result: GENOTOXIC EFFECTS:
- With and without metabolic activation: no increase in reverse mutation rate in any of the treated groups. Positve controls showed an appropriate increase in mutation rate.

PRECIPITATION CONCENTRATION: none reported.
CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: none observed at the highest test concentration of 5000 ug/plate.

Source: Huntingdon Life Sciences Ltd 1996k.
Hayes Consultancy Service Bromley, Kent
Test condition: SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA98 and TA100
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9 Arocholor 1254 induced.

ADMINISTRATION:
- Dosing: 50, 158, 500, 1580 and 5000 ug/plate.
- Number of replicates: Duplicate
- Application: Pour plate, solvent DMSO.
- Positive and negative control groups and treatment: Negative controls DMSO and untreated bacterial control. Positive controls benzo[a]pyrene 5 ug/plate, sodium azide 2 ug/plate, 2-nitrofluorene 1 ug/plate.
- Incubation: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: not reported
Test substance: Tradename Kalcol 0898
Conclusion: The C8 alcohol Kalkohl 0898 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to and including 5000 ug/plate.
Reliability: (2) valid with restrictions
Ames test no protocol specified but similar OECD 471 using only 2 tester strains. Criteria for evaluation were not

reported.
Flag: Critical study for SIDS endpoint
Reference: Huntingdon Life Sciences Ltd. 1996k. Kalcohl 0898: Preliminary toxicity screen: Assessment of mutagenic potential in histidine auxotrophs of Salmonella typhimurium (the Ames test). Final report. Report No. 96/KAS216/0148.
17-OCT-2004 (61)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Type: other: Bacterial reverse mutation assay (Ames test)
System of testing: Salmonella typhimurium strains TA98 and TA100
Concentration: 0.5 to 50 ug/plate
Cytotoxic Concentration: Slight thinning of background lawn at 50 ug/plate.
Metabolic activation: with and without
Result: negative

Method: other: Ames
Year: 1996
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)

Result: GENOTOXIC EFFECTS:
Preliminary study - Preliminary study without metabolic activation - At dose levels of 250 ug/plate and above there was an absence of revertant colonies with background lawn thin or absent. At 50 ug/plate there was slight thinning of background lawn with good population of revertant colonies. At 25 ug/ml there was no thinning of background lawn.

Main study - With and without metabolic activation: no increase in reverse mutation rate at any test concentration. All positive and negative controls showed an appropriate response.
PRECIPITATION CONCENTRATION: None reported.

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: A slight thinning of the bacterial lawn was observed at 50 ug/plate.
Source: Huntingdon Life Sciences Ltd 1996l.

Hayes Consultancy Service Bromley, Kent
Test condition: SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA98 and TA100
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9 Arocholor 1254

induced.

ADMINISTRATION:
- Dosing: 0.5, 1.6, 1.8, 5 and 50 ug/plate. Dose selection was based on a preliminary toxicity screen with TA98 in which dose levels up to 5000 ug/plate were tested.
- Number of replicates: Duplicate
- Application: Pour plate, solvent DMSO.
- Positive and negative control groups and treatment: Negative controls DMSO and untreated bacterial control. Positive controls benzo[a]pyrene 5 ug/plate, sodium azide 2 ug/plate, 2-nitrofluorene 1 ug/plate.
- Incubation: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: Not reported assume as for OECD 471

Test substance: Tradename Kalcohl 1095

Conclusion: The C10 alcohol Kalcohl 1095 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 50 ug/plate. There was evidence of cytotoxicity at the highest dose level (50 ug/plate).

Reliability: (2) valid with restrictions
Ames test no protocol specified but similar OECD 471 using only 2 tester strains. Criteria for evaluation not reported.

Flag: Critical study for SIDS endpoint

Reference: Huntingdon Life Sciences Ltd. 1996l. Kalcohl 1095: Preliminary toxicity screen: Assessment of mutagenic potential in histidine auxotrophs of Salmonella typhimurium (the Ames test). Final report. Report No. 96/KAS222/0149.

11-MAY-2006 (50)

<u>1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)</u>

Type	:	other: Bacterial reverse mutation assay (Ames Test)
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration	:	4, 20, 100, 500 and 2500 ug per plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: Henkel-method "Salmonella typhimurium reverse mutation assay" (comparable to OECD Guideline 471)
Year	:	1982
GLP	:	no

Test substance : dodecanol (112-53-8)

Test substance : Tradename Lorol 12

Test condition : METHOD Bacterial reverse mutation assay based on OECD 471. Full experimental details were not provided but actual results were available. 2-aminoanthracene was the only indicator of efficacy of the S9 mix however there was a clear increase in reverse mutation rate in bacteria treated with 2-AA in the presence of S9 compared to controls.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 0, 4, 20, 100, 500, and 2500 ug/plate aqueous suspension using Tween 80.
- Number of replicates: Four per dose level.
- Application: Plate incorporation.
- Positive and negative control groups and treatment: Positive controls were 2-amino anthracene 5 ug/plate, sodium azide 1 ug/plate; 4-nitro-o-phenylene diamine 40 ug/plate.

CRITERIA FOR EVALUATING RESULTS: Not specifically reported assume as OECD 471.

Result : GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain tested. Positive controls gave an appropriate increase in reverse mutation rate.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION:
- With metabolic activation: Total inhibition of bacterial growth at 2500 ug/plate for all strains tested except TA100 and at 500 ug/plate for TA1535 and 1537. Growth inhibition observed in TA100 at 2500 ug/plate and in all other strains at 100 or 500/plate.
- Without metabolic activation: Total inhibition of bacterial growth at 2500 and 500 ug/plate some inhibition at 100 ug/plate.

Conclusion : The C12 alcohol Lorol C12 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in

the presence or absence of metabolic activation at dose levels up to 2500 ug/plate. Cytotoxicity evidenced by complete or partial growth inhibition was observed at concentrations of >= 100 ug/plate.

Reliability	:	(2) valid with restrictions Limited documentation, in house method acceptable for assessment
Source	:	Henkel KGaA 1982b Hayes Consultancy Service Bromley, Kent
Flag	:	Critical study for SIDS endpoint
Reference		Henkel KGaA. 1982b. Dodecanol: Evaluation of mutagenicity. Unpublished data, Report No. TBD 820115.
11.08.2005		(13)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type	:	other: Bacterial reverse mutation assay (Ames Test)
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538 and E. coli WP2uvrA
Concentration	:	0.01 to 50 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: modified Ames test
Year	:	1985
GLP	:	no data
Test substance	:	dodecanol (112-53-8)
Test condition	:	METHOD Modified Ames test. SYSTEM OF TESTING - Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, TA 1538 and Escherichia coli strain WP2uvrA - Deficiences/Proficiences: Salmonella typhimurium strains histidine deficient, E. coli tryptophan deficient. - Metabolic activation system: Rat liver S9 induced with the PCB KC 500. ADMINISTRATION: - Dosing: 0.01, 0.05, 0.1, 0.5, 1, 5, 10 and 50 ug/plate. - Number of replicates: Duplicates. - Application: Preincubation method, vehicle DMSO. - Positive and negative control groups and treatment: Negative control DMSO. Postitive controls as appropriate 2-(2-furyl)-3-(5-nitro-2-furyl) acrylamide 0.01 or 0.05 ug/plate; N-ethyl-N'-nitro-N-nitrosoguanidine 5 ug/plate; 9-aminoacridine 80 ug/plate; 4-nitroquinoline-1-oxide 0.25 ug/plate; benzo[a]pyrene 5 ug/plate; 2-

aminoanthracene 5 ug/plate;
- Pre-incubation time: 20 minutes at 37C
- Incubation time: 48hours at 37C

CRITERIA FOR EVALUATING RESULTS: Not reported.

Result : GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any of the test organisms. Positive controls produced appropriate increases in mutation rate.

PRECIPITATION CONCENTRATION: None reported

CYTOTOXIC CONCENTRATION:
- With metabolic activation: >50 ug/plate (highest dose leve tested)
- Without metabolic activation: E. coli WP2 uvrA > 50 ug/plate; TA1535 10 ug/plate; other strains 50 ug/plate evidenced by growth inhibition.

Conclusion : Dodecanol did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium or tryptophan dependent E.coli WP2 uvrA in the presence or absence of metabolic activation. The material was tested to cytotoxic concentrations in the absence of S9.

Reliability : (2) valid with restrictions
Publication reporting Ames tests on various chemicals, acceptable for assessment

Source : Shimizu et al. 1985.
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Shimizu, H. et al. 1985. The results of microbial mutation test for forty-three industrial chemicals. Jpn. J. Ind. Health 27:400-419. In SIDS Dossier on 1-dodecanol. 1993.

11.08.2005 (25)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type : Bacterial reverse mutation assay

System of testing : Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, and TA 100

Concentration : 0.5 to 500 ug/plate

Cycotoxic conc. :

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 471

Year : 1996
GLP : yes
Test substance : other TS: Dodecanol CAS RN 112-53-8. Kalcohl 2098.

Test condition : SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium TA 1535, 1537, 1538, 98 and 100.
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: Based on a preliminary screening test, 0.5 (only TA1538 and 1537), 1.5, 5, 15, 50, 150 and 500 (only TA98, 100, 1535) ug/plate.
- Number of replicates: triplicates
- Application: pLate incorporation, vehicle DMSO.
- Positive and negative control groups and treatment: Negative control - vehicle (DMSO) Positive controls N-ethyl-N'-nitro-N-nitrosoguanidine 3 ug/plate (TA100) or 5ug/plate (TA1535); 9-aminoacridine 80 ug/plate (TA1537); 4-nitro-o-phenylene daimine 5 ug/plate (TA1538); 4-nitroquinoline-1-oxide 0.2 ug/plate (TA98); 2-aminoanthracene 1ug/plate TA100, 2 ug/plate (TA1535 and TA 1537), 0.5 ug/plate (TA1538 and TA98).
- Incubation: 48 hours at 37C.

DESCRIPTION OF FOLLOW UP REPEAT STUDY: Additional dose levels were tested as follows: Without S9 0.5, 1.5, 5, 15, 50 and 150 ug/plate With S9 0.5, 1.5, 5, 15, 50, 150, 500 and 1500 ug/plate. Strains TA100 and TA1538 were not tested at the two highest dose levels. The tested was replicated with extra dose levels to allow for the cytotoxicity of the test material.

CRITERIA FOR EVALUATING RESULTS: Considered positive if there is dose related and statistically significant increase in reverse mutation rate in one or more bacterial strains at sub toxic dose levels. To be considered negative the number of induced revertants should be <2 fold the number of spontaneous revertants and dose levels should extend to the limits of solubility or toxicity up to a maximum fo 5000 ug/plate.

STATISTICAL METHOD(S); Dunnetts linear regression method.

Result : GENOTOXIC EFFECTS:
With and without metabolic activation: No increase in reverse mutation rates at any test concentration. All positive and negative controls showed an appropriate response.

PRECIPITATION CONCENTRATION: An oily precipitate was observed at and above 1500 ug/plate in the preliminary toxicity assay, this did not interfere with the scoring of revertant colonies and was not reported when this dose level was tested in the repeat study.

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: The test material exhibited a visible reduction in background lawn at and above 150 ug/plate in all the strains tested. Strains TA1538, 1537 and 1535 also showed a reduction in background lawn at 50 ug/plate. This indicates that the material was tested to a toxic level.

STATISTICAL RESULTS: No statistically significant increase in reverse mutation rate at any dose level tested with or without metabolic activation.

Conclusion : The C12 alcohol Kalcohl 2098 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation. The material was tested to cytotoxic concentrations.

Reliability : (1) valid without restriction
Source : Thompson 1996a
Flag : Critical study for SIDS endpoint
Reference Thompson, P.W. 1996a. Kalcohl 2098: Reverse mutation assay "Ames test" using Salmonella typhimurium. SPL Project Number 140/590.
27.11.2003 (29)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Type: Bacterial reverse mutation assay
System of testing: Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, and TA 100
Concentration: Test 1: 15 - 5000 ug/plate; Test 2: 50 to 5000 ug/plate
Cytotoxic Concentration: >5000 ug/plate
Metabolic activation: with and without
Result: negative

Method: OECD Guide-line 471
Year: 1996
GLP: yes
Test substance: > 95% 1-Tetradecanol (112-72-1)

Result: GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in

reverse mutation rate in any strain at dose levels up to 5000 ug/plate. Positive and negative controls gave appropriate responses.

PRECIPITATION CONCENTRATION: 1500 ug/plate, plates were counted manually at this concentration and above.

CYTOTOXIC CONCENTRATION: Slight cytotoxicity was indicated in a preliminary toxicity screen with TA100 at dose levels >= 500 ug/plate without metabolic activation. In the actual mutation study there was no evidence of cytotoxicity up to 5000 ug/plate with or without S9.

STATISTICAL RESULTS: Dunnetts test was used and showed no statistically significant differences between test and control plates.

Source: Thompson 1996b.

Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

Test condition: SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 1535, TA 1537, TA 1538, TA 98, and TA 100
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: Rat liver S9 Arocholor 1254 induced

ADMINISTRATION:
- Dosing: Test 1: 15 (-S9 only), 50, 150, 500, 1500 and 5000 ug/plate. Test 2: 50, 150, 500, 1500 and 5000 ug/plate.
- Number of replicates: triplicate
- Application: Plate incorporation assay, vehicle DMSO
- Positive and negative control groups and treatment: Vehicle control- DMSO. Postive controls without S9- N-ethyl-N'-nitrosoguanidine 3 ug/plate (TA100), 5ug/plate (TA1535), 9-aminoacridine 80 ug/plate (TA1537), 4-nitro-o-phenylene diamine 5ug/plate (TA 1538), 4-nitroquinoline-1-oxide 0.2 ug/plate (TA98). with S9 2-aminoanthracene (0.5, 1 or 2 ug/plate).
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: A dose related and statistically significant increase in reverse mutation rate in one or more bacterial strains at sub-toxic dose levels. For a negative result the numbers of induced revertants should be

less than two fold compared to controls.
Test substance: Tradename Kalcol 4098.
Conclusion: The C14 alcohol Kahlcol 4098 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 5000 ug/plate. This dose level was not cytotoxic.
Reliability: (1) valid without restriction
Guideline study.
Flag: Critical study for SIDS endpoint
Reference: Thompson, P.W. 1996b. Kalcohl 4098: Reverse mutation assay "Ames test" using Salmonella typhimurium. SPL Project Number 140/597.
16-OCT-2004 (74)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: Bacterial reverse mutation assay
System of testing: Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, and TA 100
Concentration: 50 to 5000 ug/plate
Metabolic activation: with and without
Result: negative

Method: OECD Guide-line 471
Year: 1996
GLP: yes
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain at dose levels up to 5000 ug/plate. Positive and negative controls gave appropriate responses.

PRECIPITATION CONCENTRATION: 5000 ug/plate this did not interfere with counting revertant colonies.

CYTOTOXIC CONCENTRATION: There was no evidence of cytotoxicity up to 5000 ug/plate with or without S9.

STATISTICAL RESULTS: Dunnetts test was used and showed no statistically significant differences between test and control plates.
Source: Thompson 1996c.

Hayes Consultancy Service Bromley, Kent

Test condition: SYSTEM OF TESTING

- Species/cell type: Salmonella typhimurium strains TA 1535, TA 1537, TA 1538, TA 98, and TA 100
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced

ADMINISTRATION:

- Dosing: 50, 150, 500, 1500 and 5000 ug/plate for both tests.
- Number of replicates: Duplicate tests each performed in triplicate
- Application: Plate incorporation assay, vehicle acetone
- Positive and negative control groups and treatment: Vehicle control- acetone. Postive controls without S9- N-ethyl-N'-nitrosoguanidine 3 ug/plate (TA100), 5ug/plate (TA1535), 9-aminoacridine 80 ug/plate (TA1537), 4-nitro-o-phenylene diamine 5ug/plate (TA 1538), 4-nitroquinoline-1-oxide 0.2 ug/plate (TA98). with S9 2-aminoanthracene (0.5, 1 or 2 ug/plate).
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: A dose related and statistically significant increase in reverse mutation rate in one or more bacterial strains at sub-toxic dose levels. For a negative result the numbers of induced revertants should be less than two fold compared to controls.

Test substance: Tradename Kalcol 6098

Conclusion: The C16 alcohol Kahlcol 6098 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 5000 ug/plate. This dose level was not cytotoxic.

Reliability: (1) valid without restriction
Guideline study.

Flag: Critical study for SIDS endpoint

Reference: Thompson, P.W. 1996c. Kalcohl 6098: Reverse mutation assay "Ames test" using Salmonella typhimurium. SPL Project Number 140/499.

06-AUG-2005 (88)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Type: other: Bacterial reverse mutation assay screening test

System of testing: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537 and TA 1538

Concentration: 50 ug/spot
Cytotoxic Concentration: 50 ug/spot
Metabolic activation: with and without
Result: negative

Method: other: Ames et al. 1975.
Year: 1982
GLP: no data
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: GENOTOXIC EFFECTS:
- With and without metabolic activation: No evidence of increased reverse mutation in any strain in this screening (spot) test. Appropriate responses were obtained with positive and negative controls.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION: By inference a non-cytotoxic concentration (50 ug/spot) was chosen for this screening test.
Source: Blevins and Taylor 1982.

Hayes Consultancy Service Bromley, Kent
Test condition: SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537 and TA 1538
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: Spot test at a single concentration of 50 ug.
- Number of replicates: Not replicated, screening test only.
- Application: Spot test assay, vehicle sterile double distilled water.
- Positive and negative control groups and treatment: Vehicle control and 2-aminoanthracene to demonstrate activity of the S9 metabolising fraction. No other positive controls.
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: Increase in revertants over control levels, however further details were not reported.
Conclusion: Hexadecanol was evaluated in a screening test using histidine deficient strains of Salmonella typhimurium. There was no evidence of mutagenic activity with or without metabolising fraction. Results also reported in summary in CIR 1988.

Reliability: (4) not assignable
Comparative screenng study only.
Reference: Blevins, R.D. and Taylor, D.E. 1982. Mutagenicity screening of twenty-five cosmetic ingredients with the Salmonella/microsome test. J. Environ. Sci. Health A17 (2): 217-239.
11-MAY-2006 (12)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: other: Bacterial reverse mutation assay (Ames Test)
System of testing: Salmonella typhimurium strains TA 100, TA 1535, TA 1537, TA 1538, TA 98
Concentration: 4, 20, 100, 500, 2500 ug/plate
Cytotoxic Concentration: Not cytotoxic without S9, some evidence of cytotoxicity with S9 at 500 and/or 2500 ug/plate.
Metabolic activation: with and without
Result: negative

Method: other: An in-house protocol based on OECD Guide-line 471
Year: 1983
GLP: no data
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain tested. Positive controls gave an appropriate increase in reverse mutation rate.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION:
- With metabolic activation: Some evidence of a decrease in revertants at higher dose levels for TA 100 and TA 1535, effect on background lawn not reported.
- Without metabolic activation: No clear cytotoxic effect.

Source: Henkel KGaA 1981d.
Hayes Consultancy Service Bromley, Kent
Test condition: METHOD Bacterial reverse mutation assay based on OECD 471. Full experimental details were not provided but actual results were available. 2-aminoanthracene was the only indicator of efficacy of the S9 mix however there was a clear increase in reverse mutation rate in bacteria treated with 2-AA in the presence of S9 compared to controls. no repeat assay.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA

100, TA 1535, TA 1537, and TA 1538
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 0, 4, 20, 100, 500, and 2500 ug/plate aqueous suspension using Tween 80.
- Number of replicates: Duplicate.
- Application: Plate incorporation, aqueous suspension with Tween 80.
- Positive and negative control groups and treatment: Positive controls were 2-amino anthracene 5 ug/plate, sodium azide 1 ug/plate; 4-nitro-o-phenylene diamine 40 ug/plate.

CRITERIA FOR EVALUATING RESULTS: Not specifically reported assume as OECD 471.

Test substance: Tradename Lanette 16

Conclusion: The C16 alcohol Lanette 16 (Lorol 16) did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 2500 ug/plate. There was some evidence of cytotoxicity in some strains at higher dose levels (500 and/or 2500 ug/plate) in the absence of metabolising fraction. This study was also reported in summary in the Iuclid 2000 for hexadecanol.

Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

Flag: Critical study for SIDS endpoint

Reference: Henkel KGaA. 1981d. Hexadecanol: Evaluation of mutagenicity. Unpublished data, Report No. TBD 810085. (no. 236).

Iuclid 2000 European Commission - European Chemicals Bureau
Hexadecan-1-ol Cas# 36653-82-4.
06-AUG-2005 (40) (50)

<u>1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)</u>

Type	:	Bacterial reverse mutation assay
System of testing	:	Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, and TA 100
Concentration	:	50 to 5000 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative

Method	:	OECD Guide-line 471
Year	:	1996
GLP	:	yes
Test substance	:	octadecanol (112-92-5)
Test substance	:	Tradename Kalcol 8098
Test condition	:	SYSTEM OF TESTING - Species/cell type: Salmonella typhimurium strains TA 1535, TA 1537, TA 1538, TA 98, and TA 100 - Deficiences/Proficiences: Histidine deficient - Metabolic activation system: Rat liver S9 Arocholor 1254 induced ADMINISTRATION: - Dosing: 50, 150, 500, 1500 and 5000 ug/plate. - Number of replicates: Duplicate tests each performed in triplicate - Application: Plate incorporation assay, vehicle ethanol. - Positive and negative control groups and treatment: Vehicle control-ethanol. Postive controls without S9- N-ethyl-N'-nitrosoguanidine 3 ug/plate (TA100), 5ug/plate (TA1535), 9-aminoacridine 80 ug/plate (TA1537), 4-nitro-o-phenylene diamine 5ug/plate (TA 1538), 4-nitroquinoline-1-oxide 0.2 ug/plate (TA98). with S9 2-aminoanthracene (0.5, 1 or 2 ug/plate). - Incubation time: 48 hours at 37C. CRITERIA FOR EVALUATING RESULTS: A dose related and statistically significant increase in reverse mutation rate in one or more bacterial strains at sub-toxic dose levels. For a negative result the numbers of induced revertants should be less than two fold compared to controls.
Result	:	GENOTOXIC EFFECTS: - With and without metabolic activation: No increase in reverse mutation rate in any strain at dose levels up to 5000 ug/plate. Positive and negative controls gave appropriate responses. PRECIPITATION CONCENTRATION: >=500 ug/plate but this did not interfere with scoring of the plate, plates were counted manually at 5000 ug/plate. CYTOTOXIC CONCENTRATION: There was no evidence of cytotoxicity up to 5000 ug/plate with or without S9. STATISTICAL RESULTS: Dunnetts test was used and showed no statistically significant differences between test and control plates.
Conclusion	:	The C18 alcohol Kahlcol 8098 did not increase the reverse mutation

rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 5000 ug/plate. This dose level was not cytotoxic.

Reliability : (1) valid without restriction
Guideline study
Source : Thompson 1996d
Hayes Consultancy Service Bromley, Kent
Flag : Critical study for SIDS endpoint
Reference Thompson, P.W. 1996d. Kalcohl 8098: Reverse mutation assay "Ames test" using Salmonella typhimurium. SPL Project Number 140/505.
12.08.2005 (24)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Type : other: Bacterial reverse mutation assay (screening test)
System of testing : Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537
Concentration : 3 µmol/plate (spot test)
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: Ames test
Year : 1980
GLP : no
Test substance : octadecanol (112-92-5)

Test condition : SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced. Activity tested using 2-aminoanthracene.

ADMINISTRATION:
- Dosing: 3 umol/plate
- Number of replicates: not reported
- Application: Spot test screening only
- Positive and negative control groups and treatment: 2-aminoanthracene and N-methyl-N'-nitrosoguanidine.

CRITERIA FOR EVALUATING RESULTS: Not reported.

Result : GENOTOXIC EFFECTS:
- With or without metabolic activation: Reported as not mutagenic but precipitation of the test material made the results difficult to evaluate.

PRECIPITATION CONCENTRATION: 3 umol/plate

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: No significant cytotoxicity at the concentration tested.

Conclusion : This test with octadecanol is a screening test and of limited value especially as precipitation made interpretation difficult. However the test was reported as negative.

Reliability : (3) valid with restrictions
Publication, results reported for a number of chemicals including octadecanol, limited data presented.

Source : Florin, 1980

Hayes Consultancy Service Bromley, Kent

Reference

Florin, I.; Rutberg, L., Curvall, M. and Enzell, C.R. 1980. Screening of tobacco smoke constituents for mutagenicity using the Ames' test. Toxicology 18: 219-232, 1980.

SIDS Dossier on 1-Octadecanol. 1993b. Environmental Protection Agency, Denmark. 6 June 1993.

12.08.2005 (7) (23)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Type : other: bacterial reverse mutation assay screening test
System of testing : Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, and TA1538
Concentration : 50 ug/spot
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: Ames et al, 1975
Year : 1982
GLP : no
Test substance : octadecanol (112-92-5)

Test condition : SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537 and TA 1538
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:

- Dosing: Spot test at a single concentration of 50 ug.
- Number of replicates: Not replicated, screening test only.
- Application: Spot test assay, vehicle sterile double distilled water.
- Positive and negative control groups and treatment: Vehicle control and 2-aminoanthracene to demonstrate activity of the S9 metabolising fraction. No other positive controls.
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: Increase in revertants over control levels with significant dose-related increase over controls.

Result : GENOTOXIC EFFECTS:
- With and without metabolic activation: No evidence of increased reverse mutation in any strain in this screening (spot) test. Appropriate responses were obtained with positive and negative controls.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION: By inference a non-cytotoxic concentration (50 ug/spot) was chosen for this screening test.

Conclusion : Stearyl aclohol (C18) was evaluated in a screening (spot) test using histidine deficient strains of Salmonella typhimurium. There was no evidence of mutagenic activity with or without metabolising fraction.

Reliability : (4) not assignable
Publication, results reported for a number of chemicals including octadecanol, acceptable for assessment.

Source : Blevins et al, 1982
Hayes Consultancy Service Bromley, Kent

Reference
12.08.2005

Blevins, R.D. and Taylor, D.E. 1982. Mutagenicity screening of twenty-five cosmetic ingredients with the Salmonella/microsome test. J. Environ. Sci. Health A17 (2): 217-239.

SIDS Dossier on 1-Octadecanol. 1993b. Environmental Protection Agency, Denmark. 6 June 1993.
(3) (23)

<u>1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)</u>

Type : Bacterial reverse mutation assay
System of testing : Salmonella typhimurium strains TA1535, TA1537, TA 1538, TA98, TA100

Concentration	:	0.63, 1.25, 2.5, 5, 10 and 20 µg/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: Ames test (Japanese Ministry of Labour protocol)
Year	:	1982
GLP	:	no data
Test substance	:	octadecanol (112-92-5)
Test substance	:	Octadecanol CAS RN 112-92-5 (Kalcohl 80, 718)
Test condition	:	SYSTEM OF TESTING - Species/cell type: Salmonella typhimurium strains TA1535, TA1537, TA 1538, TA98, TA100 - Deficiences/Proficiences: Histidine deficient - Metabolic activation system: rat liver cells, KC500 induced... ADMINISTRATION: - Dosing: 0.63, 1.25, 2.5, 5, 10 and 20 µg/plate - Number of replicates: Single test performed in duplicate. - Application: Vehicle DMSO - Positive and negative control groups and treatment: Positive controls: N-ethyl-N'-nitro-N-nitrosoguanidine 10 µg/plate; 4-nitroquinoline 0.5 µg/plate; 2-nitrofluorene 5 µg/plate; 9-aminoacridine 50 µg/plate; 2-aminoanthracene 2 µg/plate. Not stated whether the controls were untreated or solvent controls. - Incubation time: preincubation for 20 minutes, incubation of plats for 48 hours. CRITERIA FOR EVALUATING RESULTS:
Result	:	GENOTOXIC EFFECTS: - With and without metabolic activation: No increase in reverse mutation rate. PRECIPITATION CONCENTRATION: None reported. CYTOTOXIC CONCENTRATION: Test concentrations were determined by solubility in phosphate buffer at the preincubation stage. There was no significant reduction in background lawn.
Conclusion	:	The stearyl alcohol (Kalcohl 80, 718) did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at

dose levels determined bu solubility up to 20 µg/plate. There was no evidence of cytotoxicity

Reliability : (2) valid with restrictions
Publication, acceptable for assessment.

Source : Hachiya, 1982
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Hachiya, N.; Takeya, A.; Takizawa, Y. 1982. Japanese J. Public Health 29(5): 236-239, 1982 (In Japanese, translation available).

SIDS Dossier on 1-Octadecanol. 1993b. Environmental Protection Agency, Denmark. 6 June 1993.

12.08.2005 (8) (23)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Remark: The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5- to C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C20 (eicosanol) alcohol are available from studies of reliability 1 or 2 for hexadecanol, octadecanol [Ames] and docosanol [Ames, gene mutation, chromosome abberation].

Test substance: >= 90% 1-eicosanol (629-96-9)

Conclusion: Not expected to be genotoxic in vitro.

Reliability: (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

15-SEP-2005 (18) (23)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Type: Salmonella typhimurium reverse mutation assay

System of testing: S. typhimurium strains TA-1535, -1537, -1538, -98, -100

Concentration: 10, 100, 333, 667, and 1000 µg/plate
Cytotoxic Concentration: >1000 µg/plate
Metabolic activation: with and without
Result: negative

Method: other: similar to OECD 471
Year: 2002
GLP: no data
Test substance: >95% 1-docosanol (661-19-8)
Result: GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain tested at concentrations up to 1000 ug/plate. Positive and negative controls gave appropriate responses.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION: Assume >1000 µg/plate as dose levels were based on a cytotoxicity screen.
Source: Iglesias, 2002a
Hayes Consultancy Service Bromley, Kent
Test condition: METHOD S. typhimurium reverse mutation assay. Carried out at a contract laboratory in Germany. This appears to be a standard OECD 471 assay although not all details are given in the publication.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA-1535, -1537, -1538, -98, -100
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9

ADMINISTRATION:
- Dosing: 10, 100, 333, 667, and 1000 ug/plate based on a toxicity screen.
- Number of replicates: Two tests carried out each in triplicate
- Application: Plate incorporation assay, vehicle ethanol
- Positive and negative control groups and treatment: Negative: untreated and vehicle controls. Positive: Sodium azide , 4-nitro-O-phenylene diamine, 2-aminoanthracene.

CRITERIA FOR EVALUATING RESULTS:For a test to be considered positive there should be either a two fold (TA 100) or three fold (other strains) increase in reverse mutation rate or a dose related increase in revertants.

Test substance: C22 alcohol CAS RN 661-19-8 [Behenyl alcohol]
Conclusion: Behenyl alcohol (C22) did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to and including 1000 ug/plate.
Reliability: (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).
Flag: Critical study for SIDS endpoint
Reference: Iglesias, G, JJ Hlywka, JE Berg, MH Khalil, LE Pope and D Tamarkin. 2002a. The toxicity of behenyl alcohol: I. Genotoxicity and subchronic toxicity in rats and dogs. Regulatory Tox. and Pharm. 36, 69-79.
06-AUG-2005 (15)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Type: Ames test
System of testing: Salmonella typhimurium strains TA98 and TA100
Concentration: 0, 50, 150, 500, 1000 and 5000 ug/plate
Cytotoxic Concentration: >5000 ug/plate
Metabolic activation: with and without
Result: negative

Method: other: method K709.03 (Ames test)
Year: 1997
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)

Result: GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in either strain at dose levels up to 5000 ug/plate. Positive and negative controls gave appropriate responses.

PRECIPITATION CONCENTRATION: >=500 ug/plate but this did not interfere with scoring of the plates.

CYTOTOXIC CONCENTRATION: There was no evidence of cytotoxicity up to 5000 ug/plate with or without S9.

STATISTICAL RESULTS: Dunnetts test was used and showed no statistically significant differences between test and control plates.
Source: Thompson, 1997
Hayes Consultancy Service Bromley, Kent
Test condition: SYSTEM OF TESTING

- Species/cell type: Salmonella typhimurium strains TA 98 and TA 100
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: Rat liver S9 Arocholor 1254 induced

ADMINISTRATION:
- Dosing: 50, 150, 500, 1500 and 5000 µg/plate.
- Number of replicates: Single test performed in duplicate
- Application: Plate incorporation assay, vehicle tetrahydrofuran.
- Positive and negative control groups and treatment: Vehicle control- tetrahydrofuran. Postive controls without S9- N-ethyl-N'-nitrosoguanidine 3 µg/plate (TA100), 4-nitroquinoline-1-oxide 0.2 µg/plate (TA98). with S9 2-aminoanthracene (0.5 or 1 µg/plate).
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: A dose related and statistically significant increase in reverse mutation rate in one or more bacterial strains at sub-toxic dose levels. For a negative result the numbers of induced revertants should be less than two fold compared to vehicle controls.

Test substance: Tradename Kalcol 220-80

Conclusion: Kalcol 220-80 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 5000 µg/plate. This dose level was not cytotoxic.

Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions (only 2 strains and test not repeated).

Flag: Critical study for SIDS endpoint

Reference: Thompson, P.W. 1997 Kalcol 220-80: Reverse mutation assay "Ames test" using Salmonella typhimurium strains TA98 and TA100 - Single experiment SPL Project Number: 140/723.

06-AUG-2005 (27)

<u>1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)</u>

Remark: 1-Triacontanol was negative for mutagencity in an Ames test. No further details available.

Reliability: (4) not assignable

Reference: EPA (1983). US Environmental Protection Agency. Tolerances and Exemptions from Tolerances for Pesticide Chemical in or on Raw Agricultural Commodities: 1-Triacontanol. Fed. Reg. 48, (92), 21132.

05-APR-2007

5.5 Genetic Toxicity 'in Vitro' (Non-bacterial Test)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Chromosomal aberration test
System of testing	Human peripheral lymphocyte
Test concentration	1 % v/v
Cycotoxic concentr.	Not recorded
Metabolic activation	without
Result	negative
Method	other
Year	1985
GLP	no data
Test substance	other TS: analytical grade ethanol (64-17-5)
Method	No of replicates: 2 (as solvent control to two other substances). Duration of treatment: 24 hours. Number of metaphases analyzed: 100 or 200. In vitro actication, chromosomal aberrations in blood cultures (without and with S9 mix delivered via an improvised dialysis bag); sister chromatid exchange and C-mitotic effects and polyploidies in blood cultures were studied.
Remark	All compounds produced C-mitoses, polyploidies and micronuclei. the latter interpreted as resulting from errors in the anaphase distribution of chromosomes by spindle disturbances rather than from structural chromosome aberration.
Result	Ethanol produced 3 aberrations in 100 metaphases in one study and 4 aberrations in 200 meta phases in another study.
Reliability	(2) valid with restrictions This study appears to be well conducted with appropriate controls. The study is regarded as valid with restrictions.
Flag	Critical study for SIDS endpoint
Reference	Banduhn, N. and Obe, G. (1985). Mutagenicity of methyl-2-benzimidazole, diethylstilboestrol and estradiol: Structural chromosomal aberrations, sister chromatid exchanges, C-mitoses, polyploidies and micronuclei. Mutat. Res. 1985; 156: 199-218.
12.11.2004	(227)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Chromosomal aberration test
System of testing	Chinese hamster ovary cell
Test concentration	5%
Cycotoxic concentr.	>5%

Metabolic activation	no data
Result	negative
Method	other

Year	1989
GLP	no data
Test substance	ethanol (64-17-5)

Method	This study examined the potentiating effect of ethanol on other clastogens in Chinese hamster ovary cells in vitro. Plating rate: 3x10"5 cells per petri dish. Number of replicates: not given. Frequency of dosing: single dose for 3 hrs. Positive controls: Methyl methanesulphonate, bleomycin, mitomycin. Number of metaphases analysed: 100-200 per treatment. Information cited on aberrant metaphases, chromatid breaks and exchanges, chromosome types (break or rlngldicentric). Solvent: double distilled water. Statistical methods: chi-square analysis to assess if effects between two treatments give statistically significant differences.
Result	Treatment with ethanol alone (5% for 3 hours) had no clastogenic activity as demonstrated in lack of induction of chromosome breaks and chromatid exchanges. Tabulated data is reported for 0 and 4% ethanol. Ethanol was found to potentiate the clastogenicity of known clastogens (those used as positive controls) with a clear dose response relationship.
Test Substance	Absolute ethanol (ex Merck)
Reliability	(2) valid with restrictions Key data that would be required to assess compliance with the OECD protocol are not reported in this study. However, it does appear to be otherwise reliable.
Reference	Un, Y-C., Ho, I-C., lee, T-C. (1989). Ethanol and acetaldehyde potentiate the c1astogenicity of ultraviolet light, methane methanesulfonate, mitomycin C and bleomycin in Chinese hamster ovary cells. Mutat. Res. 216: 93-99.
12.11.2004	(228)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Cytogenetic assay
System of testing	human lymphoblastoid cells
Test concentration	1% and 2%
Cycotoxic concentr.	Not stated
Metabolic activation	no data

Result	negative
Method	other
Year	1992
GLP	no data
Test substance	ethanol (64-17-5)
Method	This study involved ethanol (1% or 2%) alone as a control in an interaction study to evaluate the effect of ethanol on lobeline sulfate and bleomycin. Two cell lines evaluated, one derived from a female with multiple primary malignancies and the second from a patient with cutaneous melanoma. Number of replicates: 3 Frequency of dosing: no data Controls: negative and positive (bleomycin) Number of metaphases analysed: 100. Solvent: no data, presumed water. Statistical method: student t test. Results quoted as number of chromatid breaks per cell, with comparison made with cultures with no treatment.
Result	Ethanol (1%) alone showed breakage rates not significantly different from controls.
Reliability	(4) not assignable Study reasonably well reported. Study not designed primarily to assess clastogenicity of ethanol and some details, required to assess compliance with OECD protocol, are not reported. Appears to be reliable with restrictions.
Reference	Brown, N.M., Trizna, Z., Pathak, S. (1992). Clastogenic interactions between lobeline sulfate and ethyl alcohol: A cytogenetic study. Anticancer Research 1992; 12: 1467-1470.
12.11.2004	(229)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Cytogenetic assay
System of testing	mouse embryo
Test concentration	22, 65, 220 and 650 mM plus control
Cycotoxic concentr.	
Metabolic activation	no data
Result	negative
Method	other
Year	1991
GLP	no data
Test substance	ethanol (64-17-5)

Method	This study investigated whether acetaldehyde, the primary metabolite of ethanol, is responsible for evoking the obselVed embryotoxicity, embryolethality, chromosome-breaking activity and induction of sister chromatid exchange in mouse embryos in vitro. 4-Methylpyrazole was used to inhibit alcohol dehydrogenase. It is shown that mouse oocytes as well as morulae and blastocysts are able to xidise ethanol in the presence of NAD+
Result	Embryotoxicity in pre-implantation embryos was due to acetaldehyde.
Reliability	(4) not assignable
Reference	Lau, C-F., Vogel, R., Obe, G., Spielmann. H. (1991). Embryologic and cytogenetic effects of ethanol on preimplantation mouse embryos in vitro. Reproductive Toxicology 1991; 5: 405-410.
12.11.2004	(230)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Cytogenetic assay
System of testing	human lymphoid cells
Test concentration	2%, 4%, 6%, 8% and 10%
Cycotoxic concentr.	8% and 10%
Metabolic activation	no data
Result	positive
Method	other
Year	1991
GLP	no data
Test substance	ethanol (64-17-5)
Method	This study was part of a cocarcinogen evaluation involving cigarette smoke condensates in vitro. Concentrations of ethanol were included as controls. Ethanol alone showed no demonstrable c1astogenic activity as measured by the frequency of chromatid breaks per cell. At relatively high doses (below cytotoxic doses of 8% and 10%) ethanol inhibited DNA and chromosome repair systems. At 4% there was pronounced uncoiling of chromatids and at 6% the uncoiling was difficult to identify mitotic figures.
Reliability	(4) not assignable
Reference	Hsu, T.E., Furlong, C., Spitz, M.R. (1991). Ethyl alcohol as a cocarcinogen with special reference to the aerodigestive tract: A cytogenetic study. Anticancer Research 1991 ;11: 1097-1102.
12.11.2004	(231)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Cytogenetic assay
System of testing	Human lymphocytes
Test concentration	0.8 and 1% ethanol (equivalent to 6.31 and 7.89 mg/ml respectively)
Cycotoxic concentr.	
Metabolic activation	without
Result	negative
Method	other
Year	1984
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Peripheral lymphocytes were exposed to ethanol for 24 hours and 100 meta phases were analyzed per treatment.
Result	There was no increase in either chromatid breaks or isochromatic lesions at 0.8 or 1% ethanol.
Reliability	(4) not assignable
Reference	Koenigstein, M., Larisch, M., Obe, G. (1984). Mutagenicity of antiepileptic drugs I. Carbamazepine and some of its metabolites. Mutat. Res. 139; 83-86.
12.11.2004	(232)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Cytogenetic assay
System of testing	Human lymphocyte and Chinese Hamster Ovary cells
Test concentration	0.5 to 10 mg/ml
Cycotoxic concentr.	
Metabolic activation	with and without
Result	ambiguous
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Method	Human lymphocytes and Chinese hamster ovary cells were grown for 12 to 48 hors in the presence of 0.5 to 10 mg/ml in the absence or presence of S9 liver homogenate.
Remark	This paper is only an abstract.
Result	CHO cells in SP metabolised ethanol to acetaldehyde. Acetaldehyde produced a dose-dependent increase in chromosome

	damage below 5 mglml in the same study.
Reliability	(4) not assignable
Reference	Au, W. and Badr, F.M. (1979) Does ethanol induce chromosome damage. In vitro 15, 221.
12.11.2004	(233)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Cytogenetic assay
System of testing	Chinese hamster ovary cells
Test concentration	160 mmol/l (equivalent to 7.37 mg/ml)
Cycotoxic concentr.	
Metabolic activation	without
Result	negative
Method	other
Year	1987
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Cells were incubated with ethanol for 30 minutes at 30 degree C. 100 cells were scored for chromosome aberrations. Controls contained 3% DM50.
Result	No increase in chromosome aberrations was seen in the absence of a metabolic activation system. The S2 fraction from Zea mays induced chromosome aberrations (gaps, breaks and exchanges) when tested on the cells in the absence of ethanol. In the presence of ethanol and S2 fraction, the aberration rate was increased.
Reliability	(4) not assignable
Reference	Darroudi, F. & Natarajan, A.T. (1987). Induction of chromosomal aberrations and sister chromatid exchanges in CHO cells by mutagenic metabolites activated by plant microsomal extracts. Biologisches Zentralblatt 106: 169-174.
12.11.2004	(234)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Chromosomal aberration test
System of testing	human lymphocytes
Test concentration	25,150 and 500 mg/100 ml
Cycotoxic concentr.	

Metabolic activation	without
Result	negative
Method	other
Year	1973
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Blood obtained fron 6 men and 4 women and serum was cultured in the presence of 25 mg, 150 mg or 500 mg/100 ml ethanol for 3 days. Cells from each culture were examined for chromosome gaps, breakages, rearrangements and aneuploidy. Blastic transformation was studied by Thomas' method.
Result	Ethanol had no effect on chromosomes in vitro.
Reliability	(4) not assignable
Reference	Cadotte, M., Allard, S., Verdy, M. (1973). Lack of effect of ethanol in vitro on human chromosomes. An. Genet 16 (1): 55-56.
12.11.2004	(235)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Cytogenetic assay
System of testing	Human lymphocytes
Test concentration	1.16, 2.32, 3.48 mg/ml
Cycotoxic concentr.	
Metabolic activation	without
Result	positive
Method	other
Year	1977
GLP	no data
Test substance	ethanol (64-17-5)
Remark	A significant dose-related increase ($p < 0.05$) in chromosome aberrations (particularly chromatid and chromosome gaps and breaks) was seen at all dose levels.
Result	Cells from 5 donors incubated with ethanol for 50 hours. 100 metaphases/donor screened for chromosome aberrations.
Reliability	(4) not assignable
Reference	Badr, F.M. et al. (1977) Evaluation of the mutagenic effects of alcohol by different techniques. Adv. Exp. Med. Biol. 85a, 25 - 46.
12.11.2004	(236)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Mouse lymphoma assay
System of testing	Mouse lymphoma
Test concentration	L5178Y cells, TK +10.092,0.184,0.369,0.553,0.738 mol/l without activation; 0.414, 0.465 and 0.517 mol/l with activation
Cycotoxic concentr.	Maximum concentration with metabolic activation caused <10% fall in growth
Metabolic activation	with and without
Result	negative
Method	other: Clive et a1. (1979)
Year	1988
GLP	no data
Test substance	ethanol (64-17-5)
Method	Test design: mouse lymphoma cell TK +1- forward mutation assay with and without metabolic activation. No. of replicates: 3 per dose level but 6 for negative control. Frequency of dosing: One 4 h exposure. Positive and negative controls: Negative (no ethanol) only. Number of metaphases analyzed: Not relevant. Solvent Vehicle: Not discussed. Follow up: Not relevant. Criteria for evaluating results: 2-fold or greater increase in mutation frequency at 10% or greater total growth ct. controls. Statistical test 2-tailed Student's t-test.
Remark	Results are supported by those of Amacher, D., et al. (1980) Mutat. Res. 72:447-474. Test specific confounding factors: None. Dose-effect related observations: No clear-cut dose-effect related observations were seen. Frequency of reversions etc.: Without activation, mutation index values from lowest to highest dose were 1.3, 1.1, 1.2, 1.1 and 1.6. With metabolic activation these values were 1.1, 1.3 and 1.8. Mitotic index: Not strictly applicable. Total growth cf. controls were 88, 84, 53, 34 and 17% from lowest to highest concentrations in the absence of activation. With activation, total growth was 43, 24 and 6% from lowest to highest concentration.
Result	Only at the maximum concentration, with metabolic activation was total growth <10% control. Without activation, the lowest and highest concentrations of ethanol produced statistically significant increases in mutation frequency.

	See Remarks.
Conclusion	Ethanol is judged not to have significant mutagenic activity in this system.
Reliability	(2) valid with restrictions
Reference	Wangenheim. J. and Bolcsfoldi, G. (1988). Mouse lymphoma L5178Y thymidine kinase locus assay of 50 compounds. Mutagen. 3(3):193-205.
12.11.2004	(237)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Mouse lymphoma assay
System of testing	Mouse lymphoma L5178Y cells, TK +/-
Test concentration	Up to 7.79 x 10^{-1} M (equivalentto ca. 35.9 mg/ml)
Cycotoxic concentr.	More than 2%
Metabolic activation	without
Result	negative
Method	other
Year	1980
GLP	no data
Test substance	ethanol (64-17-5)
Method	Cells determined free of mycoplasma before use. Stock cells treated weekly with THMG mixture to reduce spontaneous mutant levels. No. of replicates: 3 Plates each and two controls Frequency of dosing: Once. Positive and negative controls: Positive controls were included. 10 Noncarcinogens and 13 putative animal carcinogens were tested. Solvent used: none. Criteria for evaluating results: Gene mutation at the thymidine kinase (TK) locus in trifluorothymidine-resistant L5178Y mouse lymphoma cells. Cytotoxicity test: 6x10E5 cells/ml suspension, 5 log range of concentrations used as range finder. Estimated 1050 used as median dose for main study. Protocol: 3 hours treatment followed by cell washing. Cell counts at 24 and 48 hours. Mutagenicity test protocol: As cytotoxicity test then split with cells resuspended in soft agar cloning medium, with or without trifluorothymidine.
Remark	Mouse lymphoma thymidine kinase assay, as described in

Amacher, O.E.
et al. (1979) Point mutations at the thymidenekinase locus in L5178Y mouse lymphoma cells. I. Application to genetic toxicology testing.
Mutation Res., 64, 391 - 406.

Result

Concentration	Cell survival	Mutants/10E4 survivors
0	100%	0.73
0.173	91 %	0.69
0.26	82%	0.77
0.346	81%	0.81
0.433	75%	0.74
0.52	63%	0.92
6.06	52%	0.68
6.93	36%	0.60
7.79	3%	0.72

No increase in mutants at clearly cytoxic concentrations.

Test Substance Purity not specified
Reliability (2) valid with restrictions
Reference Amacher, D.E. et al. (1980) Point mutations at the thymidinekinase locus in L5178Y mouse lymphoma cells. II. Test validation and interpretation. Mutation Res. 72, 447 - 474.
12.11.2004 (238)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type Mammalian cell gene mutation assay
System of testing S49 mouse lymphoma cells
Test concentration 1%

Cycotoxic concentr.
Metabolic activation with
Result negative
Method other

Year 1983
GLP no data
Test substance ethanol (64-17-5)

Method This study evaluated ethanol as the solvent control in a study of the induction of dexamethasone, 6-thioguanine and ouabain resistance.

Materials:
Dulbecco's modified Eagle's medium with 4.59 glucose/I, heat

inactivated horse serum and fetal calf serum, Bacto Agar,ICR 191 and ethanol ex Sigma. S49.1 ML cells from P Coffino, San Francisco, originally isolated by Horibata and Harris (1970).

Cells grown in stationary medium without antibiotics at 37C in a humidified C02 incubator. Freshly cloned cultures frozen at -80C. Stock cultures frequently discarded and repaced with thawed frozen ones to prevent build up of mutants. Cells stained with trypan blue for counting.

Mutagenic treatment and selection:
4 hour treatment. Cells (6x1 OE6/dose) centrifuged and re-suspended in medium containing S9. Maximum solvent concentration 1 %. Positive control used.

Criteria for positive result: survival >=40%, factor by which frequency elevated compared to control >3, frequency of 6-TG mutants elevated against controls.

Result The dexamethasone resistance marker was induced at the highest frequency and was expressed within 3 days after mutagenesis. Ethanol had no effect on the mutagenesis of this marker.

Surviving fraction: 100% Mutant frequency: 0 Mean and standard deviation of control: 104 +/- 9 Elevation of mutant freq. compared to control: 0

Reliability (2) valid with restrictions

Reference Friedrich, U., Nass, G. (1983). Evaluation of a mutation test using S49 mouse lymphoma cells and monitoring simultaneously the induction of dexamethasone resistance, 6-thioguanine resistance and ouabain resistance. Mutat. Res. 1983; 110: 147-162.

12.11.2004 (239)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type Micronucleus test
System of testing In vitro Male Chinese hamster lung fibroblast (V79) cells
Test concentration 50 microlitre/ml

Cycotoxic concentr.
Metabolic activation without
Result negative
Method other

Year 1984
GLP no data
Test substance ethanol (64-17-5)

Method	This study evaluated the micronucleus assay by comparison with sister chromatid exchange results for known mutagens/carcinogens. Ethanol, methanol, butanol and propanol were also examined. Micronucleus induction was studied in vitro in cells treated with ethanol (50 microliter/ml) for 1 hour.
Result	No significant induction of micronuclei was evoked by ethanol in V79 Chinese hamsetr cells.
Test Substance	Absolute ethanol.
Reliability	(4) not assignable
Reference	Lasne, C., Gu, Z.w., Venegas, W., Chouroulinkov, I. (1984) The in vitro micronucleus assay for detection of cytogenetic effects induced by mutagen-carcinogens: comparison with the in vitro sister-chromatid exchange assay. Mutat. Res. 130; 273-282.
12.11.2004	(240)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Sister chromatid exchange assay
System of testing	Chinese hamster ovary cells
Metabolic activation	Negative
Result	
Method	
	1977
Year	no data
GLP	95 – 99.9% ethanol (64-17-5)
Test substance	
Method	Methanol, ethanol (0.1% w/v), propanol, butanol and acetaldehyde (0.0005% and 0.001 % w/v) were evaluated for effect on SCE in CHO cells in vitro.
Result	SCE in ethanol treated cells occurred at 4.83 SCE/mitosis versus 4.52 in controls. In acetaldehyde treated cells, there were 13.56 SCE/mitosis at the lowest concentration and 28.25 SCE/mitosis at the highest concentration versus 4.69 SCE/mitosis in controls.
Conclusion	It is acetaldehyde rather than ethanol responsible for an increase in SCE in CHO cells.
Reliability	(4) not assignable
Reference	Obe, G., Ristow, H. Acetaldehyde, but not ethanol, induces sister chromatid exchanges in Chinese hamster cells in vitro. Mutat Res 1977; 56: 211-213.
12.11.2004	(241)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol, from Prolabo (Paris, France)
Type of cell used: Chinese Hamster Lung Fibroblast Cell Line (V79)

Test method: Micronucleus:
Cells treated with test material for I-hour, treated with BrdUrd (bromodeoxyuridine) for 7 hours and incubated for 48 hours (2nd cell cycle). 7000 interphase cells scored per treatment. No activation used. Solvent control = acetone.
GLP: No

Test results: Lowest Concentration producing cell toxicity:
with metabolic activation: no activation used without metabolic activation: 50 µ1/ml
Genotoxic effects:

	+	?	-
with metabolic activation:	[ ]	[ ]	[ ]
without metabolic activation:	[ ]	[ ]	[X]

Comments: No evidence of mutagenic activity in micronucleus assay using CHL V79 Cell Line at concentrations up to 50 µl/ml.
Number of micronuclei/l000 cells (mean ± S.E.) 2.75 ± 0.48
Reference: Lasne, C., Gu, Z.W., Venegas, W. And I. Chouroulinkov (1984) "The in vitro micronucelus assay for detection of cytogenetic effects induced by mutagen-carcinogens: Comparison with the in vitro sister-Chromatid exchange assay. Mutat. Res. 130: 273-282.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Test substance: 1-Butanol
Type of cell used: Chinese hamster ovary cells (CRO)
Test method:
In vitro Sister Chromatid Exchange: Cells were treated in culture once a day for 7 days with 1-butanol to a final concentration of 0.1 %. One day after the last treatment, the cells were treated with Brdu. 20 hours later the cells were teated with co]cemid. Mitotic chromosomes were prepared 4 hours later. 100 mitoses were examined for SCEs.
GLP: No

Test results: Lowest Concentration producing cell toxicity:
with metabolic activation:
without metabolic activation: >0.1% Genotoxic effects:

	+	?	-
with metabolic activation:	[ ]	[ ]	[X]
without metabolic activation:	[ ]	[ ]	[X]

Comments: No evidence of clastogenic activity in an in vitro SCE assay in CHO cells up to a concentration of 0.1 %.

Reference: Obe, G. And Ristow, H. (1977). "Acetaldehyde, but not Ethanol, Induces Sister Chromatid Exchanges in Chinese Hamster Cells in vitro." Mutat. Res. 56: 211-213.

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Remark: The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5- to C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C20 (eicosanol) alcohol are available from studies of reliability 1 or 2 for hexadecanol, octadecanol [Ames] and docosanol [Ames, gene mutation, chromosome abberation].

Test substance: as prescribed by 1.1 - 1.4

Conclusion: Not expected to be genotoxic in vitro.

Reliability: (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category
15-SEP-2005 (18) (23)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Type: Cytogenetic assay
System of testing: Chinese hamster V79 cells
Concentration: 0.6, 10.0 and 20.0 ug/ml
Cytotoxic Concentration: >20 ug/ml
Metabolic activation: with and without
Result: negative

Method: other: similar to OECD 473
Year: 2000
GLP: no data

Test substance: >95% 1-docosanol (661-19-8)

Result: GENOTOXIC EFFECTS:
- With and without metabolic activation: No relevant increases in stuructural chromosome aberrations at any dose level.

PRECIPITATION CONCENTRATION: No reported.

MITOTIC INDEX: No increase in mitotic index (results not presented in the publication)

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: No evidence of cytotoxicity at dose levels up to 20 ug/ml as evidenced by mitotic index or plating efficiency.

Source: Iglesias, 2002a
Hayes Consultancy Service Bromley, Kent

Test condition: SYSTEM OF TESTING
- Species/cell type: Chinese hamster V79 cells.
- Metabolic activation system: Rat liver S9 no other information given.
- No. of metaphases analyzed: 100 per replicate

ADMINISTRATION:
- Dosing: 0.6, 10 or 20 ug/ml for 18 hours; 20 ug/ml fo 7 or 24 hours.
- Number of replicates: Duplicates
- Application: Vehicle ethanol
- Positive and negative control groups and treatment:
- Incubation time: 7, 18 or 24 hours.

CRITERIA FOR EVALUATING RESULTS: A statistically significant dose related increase in structural chromosome aberrations or a significant postive response at one of the test points. Statistical analysis was only carried out for cells carrying aberrations-exclusive gaps. The X2 was included in the analysis.

Test substance: C22 alcohol CAS RN 661-19-8 [Behenyl alcohol]

Conclusion: Behenyl alcohol (C22) did not increase the incidence of chromosome aberrations in Chinese hamster V79 cells in the presence or absence of metabolising fraction at dose levels up to 20 ug/ml (highest dose level tested). There was no evidence of cytotoxicity at this dose level.

Reliability: (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).

Flag: Critical study for SIDS endpoint

Reference: Iglesias, G, JJ Hlywka, JE Berg, MH Khalil, LE Pope and D Tamarkin. 2002a. The toxicity of behenyl alcohol: I. Genotoxicity and subchronic toxicity in rats and dogs. Regulatory Tox. and Pharm. 36, 69-79.

06-AUG-2005 (15)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Type: Cytogenetic assay
System of testing: Chinese hamster V79 cells
Concentration: 0.6, 10.0 and 20.0 ug/ml
Cytotoxic Concentration: >20 ug/ml
Metabolic activation: with and without
Result: negative

Method: other: similar to OECD 473
Year: 2000
GLP: no data
Test substance: >95% 1-docosanol (661-19-8)

Result: GENOTOXIC EFFECTS:
- With and without metabolic activation: No relevant increases in stuructural chromosome aberrations at any dose level.

PRECIPITATION CONCENTRATION: No reported.

MITOTIC INDEX: No increase in mitotic index (results not presented in the publication)

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: No evidence of cytotoxicity at dose levels up to 20 ug/ml as evidenced by mitotic index or plating efficiency.

Source: Iglesias, 2002a
Hayes Consultancy Service Bromley, Kent

Test condition: SYSTEM OF TESTING
- Species/cell type: Chinese hamster V79 cells.
- Metabolic activation system: Rat liver S9 no other information given.
- No. of metaphases analyzed: 100 per replicate

ADMINISTRATION:
- Dosing: 0.6, 10 or 20 ug/ml for 18 hours; 20 ug/ml fo 7 or 24 hours.
- Number of replicates: Duplicates
- Application: Vehicle ethanol

- Positive and negative control groups and treatment:
- Incubation time: 7, 18 or 24 hours.
CRITERIA FOR EVALUATING RESULTS: A statistically significant dose related increase in structural chromosome aberrations or a significant postive response at one of the test points. Statistical analysis was only carried out for cells carrying aberrations-exclusive gaps. The X2 was included in the analysis.

Test substance: C22 alcohol CAS RN 661-19-8 [Behenyl alcohol]

Conclusion: Behenyl alcohol (C22) did not increase the incidence of chromosome aberrations in Chinese hamster V79 cells in the presence or absence of metabolising fraction at dose levels up to 20 ug/ml (highest dose level tested). There was no evidence of cytotoxicity at this dose level.

Reliability: (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).

Flag: Critical study for SIDS endpoint

Reference: Thompson, P.W. 1997 Kalcol 220-80: Reverse mutation assay "Ames test" using Salmonella typhimurium strains TA98 and TA100 - Single experiment SPL Project Number: 140/723.

06-AUG-2005 (15)

<u>1-Triacontanol (593-50-0) for 1-Triacontanol Aluminum Salt (67905-26-4)</u>

Test substance: 1-Triacontanol

Remark: The test substance caused chromosomal damage to the alga, *Tolypella prolifera*. No further details available.

Reliability: (4) not assignable

Reference: Bhatnager, S.K., et al. (1989). Cytologia 54, 183.
Toxicity Profile: Triacontanol. BIBRA Information Servies Ltd. Sutton, Surrey, 1997.

09-APR-2007

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5.6 Genetic Toxicity 'in Vivo'

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Micronucleus assay
Species	rat
Sex	male
Strain	other: BD6
Route of admin.	drinking water
Exposure period	10-30 days
Doses	5% or 10%
Result	negative
Method	other
Year	1993
GLP	no data
Test substance	ethanol (64-17-5)
Method	No of rats: 51 in 3 separate experiments. Weight: 180-200g Diet and drinking water: standard rodent diet; water ad libitum alone or with added ethanol. Exposure period: 10-30 days. Investigations: At end of exposure animals were killed and pulmonary alveolar macrophages and bone marrow erythroblasts were harvested. Both cytotoxic and cytogenetic effects were examined.
Remark	Assuming that rat drinking water consumption is 100ml/kg/day, 5% ethanol in drinking water would be equivalent to 5000mg/kg, well above the normal upper limit stated in DECO 474)
Result	No effect on micronucleus incidence was observed. Polynucleated PAM were enhanced. 10% dose was cytotoxic to bone marrow
Test substance	5% or 10% in drinking water as part of a co- clastogenicity study with tobacco smoke.
Reliability	(2) valid with restrictions
Flag	Critical study for SIDS endpoint
Reference	Balansky, R.M., Blagoeva, P.M., Mircheva, Z. I. and de Flora,S. Co-clastogenicity of ethanol with cigarette smoke in rat erythroblasts and anticlastogencity in alveolar macrophages. Cancer Lett 1993; 72: 183-189.
12.11.2004	(242)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Micronucleus assay
Species	rat
Sex	male
Strain	Wistar
Route of admin.	drinking water
Exposure period	3 or 6 week
Doses	10% or 20% ethanol in the drinking water given to one to four rats per dose and exposure period
Result	
Method	other
Year	1980
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Age of animals at start: Adult. No. of animals per dose: 1, 2 or 4. Dosage: 10% or 20% vlv Vehicle Control: Tap water. Duration of test: 3 or 6 weeks. Frequency of treatment: Daily Sampling: Hepatocytes, bone-marrow cells and blood lymphocytes for micronuclei, micronuclei in polychromatic erythrocytes and for sister chromatid exchanges and chromosomal aberrations. Group sizes in this study small.
Result	Negative. Drinking ethanol did not affect the incidence of micronuclei in bone marrow cells or hepatocytes at either ofthe two dose levels. Also, drinking ethanol did not affect the incidence of chromosome aberrations in bone marrow cells or cultured lymphocytes at either of the two dose levels. Frequencies of sister chromatid exchanges in blood lymphocytes are significantly enhanced in rats exposed to either dose and at the higher dose, ethanol increased the frequency of micronuclei and chromosomal aberration in polychromatic erythrocytes.
Reliability	(2) valid with restrictions
Reference	Tates, A.D. (1980) Cytogenetic effects in hepatocytes, bone-marrow cells and blood lymphocytes of rats exposed to ethanol in the drinking water. Mutation Res. 79, 285 - 288.
12.11.2004	(243)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Micronucleus assay
Species	Mouse
Sex	male

Strain	Swiss
Route of admin.	drinking water
Exposure period	27 days
Doses	up to ca. 65 g/kg body weight/day
Result	negative
Method	other
Year	1977
GLP	no data
Test substance	ethanol (64-17-5)

Method

Age at study start: 72-75 days.
No. of animals per dose: 3 in negative control, 5 in ethanol groups and 6 in positive control.
Vehicle: Water.
Duration of test: 27 days.
Frequency of treatment: Ethanol ad libitum; for positive control, ethyl methanesulfonate by injection 30 and 6 h before sacrifice.
sampling times: Sacrificed on 27th day and 4 slides of stained bone marrow taken from each mouse.
Controls: see above.
Parameters observed: Bodyweight Organs/tissues at necropsy: Bone marrow smears only.
Criteria for evaluating results: An average of 4000 polychromatic erythrocytes and corresponding normochromic cells were counted for each animal. The % of cells with micronuclei and groups means were calculated.
Criteria for selecting MTD: Not discussed. 2 animals receiving 40% over the last 2 wk died.

Remark

Age of animals at start: 72-75 days No. of animals per dose: 3 or 5
Dosage: Two gtoups of mice. Group t given 10% alcohol in the drinking water for 6 days, then 29% for 7 days followed by 30% for 14 days. Group 2 given 10% for 6 days, 30% for 7 days, then 40% for 14 days. Control group was untreated.
Duration of test: Total 26 days.
Controls: Ethyl methyl sulfonate opr dimethylsulfoxide.
Investigations: Bone marrow preparations were made and examined for polychromatic and normochromatic erythrocytes.
This investigation suffers from the limitation ofa relatively short period of alcohol ingestion. However, these data were considered sufficiently reliable by US EPAS for inclusion in the GeneTox Program report and for this reason have been assigned a reliability score of 2.
Time weighted average concentrations of ethanol were 23% and 33%.
Actual intakes were not determined.

Result

40% level in drinking water is equivalent to an intake of

approximately 65 g/kg body weight/day.

The PIN ratio was not affected by ethanol but was significantly increased in the positive (ethylmethylsulfonate) control. The incidence of micronuclei was significantly increased in the positive control group but not by ethanol.
Mortality at each dose level: 2 aniumals receiving 40% ethanol died possibly of dehydration. 2 positive control animals and 0 negative control animals died.
Mutations etc observed: The %PCE's with micronuclei in negative control, low dose, high dose and positive control groups were 0.37, 0.26, 0.24 and 0.88 respectively.
Clinical signs: Not discussed.
Body weight changes: Not affected by treatment.
Food/water consumption: Not discussed.

Test substance Test substance: "distilled ethanol".

Reliability (2) valid with restrictions

Reference Chaubey, R.C., Kavi, SR, Chauhan, P.S., Sundaram, K. (1977). Evaluation of the effect of ethanol on the frequency of micronuclei in the bone marrow of Swiss mice. Mutation Res. 43:441-444.

12.11.2004 (244)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type Cytogenetic assay
Species rat
Sex male
Strain other: CD
Route of admin. oral feed
Exposure period 6 weeks
Doses 36% of dietary energy
Result positive
Method other
Year 1981
GLP no data
Test substance ethanol (64-17-5)

Method Age of animals at start: Weanling fed until 130-150 g weight.
No. of animals per dose: 16 males per pair-fed group Rat strains: CD Dosage: 12 to 16 g/kg bodyweightlday representing 36% of total energy intake.
Duration of test: 6 weeks Frequency of treatment: Fed ad libitum in pair fed groups with group fed diet without alcohol.
Controls: Untreated only.

	Examinations: Blood samples examined for frequency of micronuclei, polychmomasia, orthochromasia. Blood ethanol concentrations were measured at Sam by tail tip excision. Statistics: student t test.
Remark	Dose of 6g/kg given by gav,agetheday before sacrifice produced no change in bone marrow cell population, mitotic index or percentage of cells with micronuclei. In the authors' opinion, the decreased proportion of nucleated cells most likely reflects hypoplasia, conceivably from cytogenetic damage of stem cells.
Result	Blood ethanol concentrations 149mg/100ml +/- 20mg. Despite pair feeding equal consumption of calories, ethanol fed animals had significantly lower bodyweight. Ethanol treatment significantly (P<0.001) decreased the number of nucleated cells per rat relative to pair-fed controls (4929 ± 774 versus 7996 ± 708) and significantly (P<0.05) increased the percentage of nucleated cells undergoing mitosis to 2.43 ± 0.47 from 1.48 ± 0.38. Ethanol significantly (P<0.001) increased the number of erythrocytes per rat from 4789 ± 525 to 7595 ± 390 with significant increases in both polychromatic and orthochromatic components. The number of erythrocytes with micronuclei, per rat, was increased significantly (P<0.01) from 35 ± 7 to 71 ± 12 of which both polychromatic and orthochromatic components were equally affected. This was also reflected in the percentage of erythrocytes with micronuclei although significant only with respect to polychromatics. Overall, the percentage of erythrocytes with micronuclei increased from 0.74 ± 0.13 ti 0.94 ± 0.16 (p<0.03) with the PCEs increaseing from 0.95 ± 0.13 to 1.30 ± 0.20 (p<0.05) and the aCEs increasing from 0.67 ± 0.12 to 0.84 ± 0.16 (not significant.)
Reliability	(2) valid with restrictions
Reference	Baraona, E., Guerra, M., Lieber, C.S. (1981). Cytogenetic damage of bone marrow cells produced by chronic alcohol consumption. Life Sci. 29, 1797-1802.
12.11.2004	(245)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Cytogenetic assay

Species	Chinese hamster
Sex	male/female
Strain	
Route of admin.	oral feed
Exposure period	9 weeks
Doses	10% v/v
Result	negative
Method	other
Year	1979
GLP	no data
Test substance	ethanol (64-17-5)
Method	Age at start of study: 10-20 weeks. Dosages: Ethanol (10%) in liquid feed (11 animals); salt water control (36 animals), cyclophosphamide (6 animals), ethanol + cyclophosphamide (8 animals); patulin (6 animals); ethanol + patulin (7 animals); aflatoxin B (10 animals) and ethanol + aflatoxin B (7 animals). Investigation: Bone marrow examined after 9 weeks for chromatid breaks, isochromatid breaks, chromatid translations and mitosis with multiple aberrations.
Result	Ethanol alone had no effect on bone marrow chromosomes in either sex.
Reliability	(2) valid with restrictions
Reference	Korte, A., Slacik-Erben, R., Obe, G. (1979). The influence of ethanol treatment on cytogenetic effects in bone marrow cells of Chinese hamsters by cyclophosphamide, aflatoxin B and patulin. Toxicology 12; 53-61.
12.11.2004	(247)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Cytogenetic assay
Species	hamster
Sex	male/female
Strain	other
Route of admin.	drinking water
Exposure period	12 week
Doses	10% in the drinking water during week 1, 15% in weeks 2 - 3, 20% in weeks 4 -12.
Result	negative
Method	other
Year	1981
GLP	no data
Test substance	other TS: Absolute, extra pure ethanol (64-17-5)

Remark	Age at study start: 10-20 weeks No. animals/dose: Ethanol treated 8 females; 9·males. Controls 9 females, 7 males. Vehicle: Water. Duration of test: 12 weeks. Frequency of treatment: Drinking water ad libitum. Controls received plain water. Diet: (Altromin 7024) Dosage: 10% v/v in the first week; 15% during the second and third week and 20% from the 4th to the 12th week. Fluid intake approximately 5.2 ml/hamster/day. Maximum intake therefore up to 26 g/kg body weight/day in males and 33 g/kg body weight/day in females. Investigations: Some animals in each group were exposed to cigarette smoke during the last 4 weeks. Bone marrow was examined for chromosomal aberrations. Ethanol also failed to induce chromosome aberrations in bone marrow cells in a similar study by the same group in which hamsters were given 10% v/v ethanol in the diet for 9 weeks (Korte, A. et al. (1979). The influence of ethanol treatment on cytogenetic effects in bone marrow cells of Chinese hamsters by cyclophosphamide, aflatoxin B1 and patulin. Toxicology 12, 53-61.
Result	2.3% aberrant metaphases detected in controls, 3.7 % in treated animals. No sex difference evident. Mitotic index significantly elevated in smoke treated group (P <0.001) but not in ethanol controls.
Reliability	(2) valid with restrictions
Reference	Korte, A., Wagner, H.M., Obe, G. (1981). Simultaneous exposure of Chinese hamsters to ethanol and cigarette smoke: cytogenetic aspects. Toxicology 20; 237-246.
12.11.2004	(248)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Cytogenetic assay
Species	hamster
Sex	male/female
Strain	other
Route of admin.	drinking water
Exposure period	46 week
Doses	10 % v/v ethanol in the drinking water given to 5 females and 2 males
Result	negative
Method	other
Year	1981

GLP	no data
Test substance	ethanol (64-17-5)
Method	Age at study start: 15 mth. Animals housed individually. No. animals/dose: Controls 3 males, 2 females. Ethanol 2 males, 5 females. Vehicle: Water. Doses were given as 10% v/v (180 g/kg/day). Duration of test: 46 wk. Frequency of treatment: Drinking water ad libitum. Controls received plain water. Sampling: Blood taken in the 47th week. Two samples per animal analyzed. Clinical obseNations: None. Organs examined at necropsy: None. Criteria for examining results: Chromosomal aberrations in lymphocytes included chromatid breaks, isochromatid breaks and chromatid translocations. An aberrant metaphase cell contained at least one aberration. Criteria for selecting MTD: None. Statistics: Chi square test.
Remark	Group size in this study was small and ingested dose was uncertain. Hamsters are reported to have ingested about 1.4:ml/g body weight/week (157g/kg body weight/week). This figure may haveqeen E;lrr9neOus as the hamsters appear to have consumed ca. 45 ml fluid/week, corresponding to an approximate intake of 17 g ethanol/kg body weight/day. The rateaf aberrant metaphases was higher in the ethanol-treated group than in the control group (10.8 versus 7.7%) but the difference was not statistically significant (p >0.25). Mortality at each dose level: None. Clinical signs: None described. Body weight changes: Did not change significantly. Food/water consumption changes: Animals consuming ethanol ate 30% less food than controls.
Test substance	Test substahce was ethanol absolute, extra pure, Merck.
Reliability	(2) valid with restrictions
Reference	Korte, A., Dbe, G. (1981). Influence of chronic ethanol uptake and acute acetaldehyde treatment on the chromosomes of bone-marrow cells and peripheral lymphocytes of Chinese hamsters. Mutation Res. 88;389-395.
12.11.2004	(249)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Dominant lethal assay
Species	mouse
Sex	male
Strain	other
Route of admin.	gavage
Exposure period	5 day
Doses	10 or 40% ethanol in water (dose volume 2 ml/kg) to groups of 15 mice
Result	ambiguous
Method	other
Year	1982
GLP	no data
Test substance	ethanol (64-17-5)
Method	Age at start of treatment: 10-12 weeks Strain: CFPL or Alderly Park. Treatment: Mice dosed with ethanol in distilled water on 5 consecutive days. Dosages: equivalent to 0.25 of the MTD (10% ethanol) and the MTD (40% ethanol). Actual doses administered were 0.16 and 0.63 g/kg body weight/day by oral gavage. Controls: treated with distilled water only. Mating: Immediately after completion of dose schedule, each male was caged sequentially with 2 undosed females each week for 8 consecutive weeks. All females were killed and examined 18 days after first being caged with males. Implantation sites and dead implants/female were recorded. Replicates: In 3 different laboratories.
Result	No effect on pregnancy rate. Occasional positive results with regard to preimplantation loss during weeks 7 and 8 (reduction in the number of implants/male). It was suggested that in most cases this was due to a lower number of implants in the corresponding control groups. There were also occasional increases in the number of postimplantation deaths/male although the majority of the post implantation results were not significant.
Conclusion	Ethanol is unlikely to be a dominant lethal mutagen, at least up to the maximum tolerated dose.
Reliability	(1) valid without restriction This is a highly reliable study that was well reported and compliant with OECD protocols
Reference	James, D.A. & Smith, D.M. (1982) Analysis of results from a collaborative study of the dominant lethal assay. Mutation Res. 97: 303-314.
12.11.2004	(250)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Dominant lethal assay
Species	mouse
Sex	male/female
Strain	Swiss
Route of admin.	other: i.p. (acute) and drinking water (chronic)
Exposure period	3 days (acute) and 11 weeks (chronic)
Doses	1.26 g/kg/day and 1.04 g/mouse/day
Result	positive
Method	other
Year	1994
GLP	no data
Test substance	ethanol (64-17-5)
Method	Age at study start: 12-16 weeks (25-30 g). Strains:. Inbred Swiss, C57Bl6 and CBA No. animals/dose: Controls 3 males, 2 females. Ethanol 2 males, 5 females. Dosage: 0.1 ml40% alcohol Lp. (acute study). 5% in drinking water increased by 5% every week to 40% and then at 40% for 4 weeks. Equivalent dose 0.13 g/mouse/day at 5%; 1.04 g/mouse/day at 40%. Period of treatment: 3 days (acute), 11 weeks (chronic). Vehicle: Water. Replicates: 2 or 3 Mating: 4-day schedule post last treatment. Investigations: Uterine contents, deciduomas, post-implantation losses.
Remark	This study was designed to reproduce the results of Badr using Lp. injection rather than intubation, but it was unable to do. The authors concluded that ethanol did not have a significant dominant lethal effect but caused some pre-implantation loss, which might be due to an effect on the fertilization capacity of sperm.
Result	In Swiss mice, the mutagenic index based on both pre- and postimplantation lethality was consistently positive. There was a marked reduction (34% and 30%) in the number of pregnant females at the first two mating times in the treated group and a significant decrease in total and live implants in the second mating. There was no increase in dead implants from the first two matings and only a small increase at the third mating (P<O.05).
Reliability	(2) valid with restrictions
Reference	Rao, U.N., Aravindakshan, M., Chauhan, P.S. (1994). Studies on the effects of ethanol on dominant lethal mutations in Swiss, C57BI6 and CBA mice. Mutat Res 1994; 311 :69-76.

12.11.2004 (251)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Dominant lethal assay
Species	mouse
Sex	male/female
Strain	C3H
Route of admin.	oral feed
Exposure period	4 weeks in males, then mated with untreated females
Doses	0%, 20% and 30% of ethanol derived calories
Result	negative
Method	other
Year	1982
GLP	no data
Test substance	other TS: 95% ethanol (64-17-5)

Method

Age at start of treatment: 10 weeks.
Strain: C3H/HE mice.
Feeding: ad libitum.
Environment: temperture and humidity controlled constant with diumal daylight/dark rhythm.
Dosage: 0%, 20% or 30% of isocaloric diet made up of ethanol-derived calories.
Replicates: pair-fed regimen.
Sampling: Weekly blood for blood alcohol concentration.
Investigations; Implantation sites, dead, resorptions and live foetuses counted.
Statistical analysis: Undernutrition and gender factors considered.

Result

No differences were found between the litters of alcohol-treated males and controls in terms of number of implantation sites, prenatal mortality, foetal weight, sex ratio or frequency of soft tissue malformations.
Paternal alcohol consumption does not grossly alter foetal growth and development in C3H mice.

Reliability (2) valid with restrictions

Reference Randall, C.L., Burling, TA, Lochry, E.A., Sutker, P.B. (1982). The effect of paternal alcohol consumption on foetal development in mice. Drug and Alcohol Dependence 9; 89-95.

12.11.2004 (252)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Dominant lethal assay
Species	mouse
Sex	male/female

Strain	other: CF1
Route of admin.	oral feed
Exposure period	5 weeks
Doses	5% v/v liquid diet (28% ethanol-derived calories)
Result	positive
Method	other
Year	1991
GLP	no data
Test substance	other TS: 95% USP ethanol (64-17-5)
Remark	Age of animals at start: 8-9 weeks; 30.1 g No. of animals per dose: 10 per group Dosage: 5% v/v in liquid diet representing 28% of total energy intake. Duration of test: 5 weeks Frequency of treatment: Fed ad libitum in pair fed groups with group fed diet with alcohol replaced by sucrose. Mating: 3 Females were housed with each male and examined daily for presence of vaginal plug to a maximum 6 days. Examinations: Tail blood samples examined for haemalocrit. Females were housed until day 14 when ovaries and uteri were scored for dominant lethal mutations. A mutation index (MI) was calculated: MI/100 = (no of corpora lutea + dead foetuses - total foetuses)/no of corpora lutea. This study was part of a co-mutagen city study involving delta-9-tetrahydrocannabinol and Trenimon.
Result	Ethanol caused minimal impairment of fertility at this dosage, but increased the frequency of dominant lethal mutations.
Reliability	(2) valid with restrictions
Reference	Berryman, S.H., Anderson Jr., R.A., Weis, J., Bartke, A. (1992). Evaluation ofthe comutagenicity of ethanol and delta-9-tetrahydrocannabinol with Trenimon. Mutat. Res. 1992; 278: 47-60.
12.11.2004	(253)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Dominant lethal assay
Species	rat
Sex	male
Strain	Sprague-Dawley
Route of admin.	oral feed
Exposure period	5 week
Doses	6% ethanol in the diet for 1 week, then 10% given to 6 rats
Result	positive
Method	other

Year	1976
GLP	no data
Test substance	ethanol (64-17-5)
Method	Animals: weight at start of treatment: 318 g (males); 259 g (females). No of animals: 12 males; 25 females. Environment: Individually housed, 22 degC, RH 45% +/-10 with diurnal light cycle (nocturnal 20:00 to 8:00hrs.) Dosage: Six treated rats were given a 6% v/v ethanol-containing liquid diet (providing 35% of calories.) This was increased to 10% vlv after 7 days exposure (58% of dietary calories. Controls: Six controls given an isocaloric amount of sucrose. Diet 'Metrecal' (chocolate or vanilla.) Duration of treatment: 15 days (males). females on lab chow and water. Investigations: After treatment each male was placed in a cage with 2 females every night. No food or water was provided during this time. The experiment was continued for 5 weeks, with the males still receiving alcohol during the day. The males were killed on day 36. Blood samples were collected. Pregnancies were terminated on day 20 of gestation and litter size and foetal mortality was assessed.
Result	Treated males showed signs of intoxication and considerable weight gain compared to controls. Treated animals were much less succesful at mating; the numbers of successful matings were 6/12 in the treated group and 13/13 in the controls. The number of offspring/litter was greater in the controls (p <0.01). A higher incidence of early resorption was seen in the treated group (p <0.01). From graphical data presented in the reference, it is possible to estimate ethanol consumption as being in the range 7.2 to 14.4 g/kg/day.
Test Substance	Test substance Was 95% v/v ethanol.
Reliability	(2) valid with restrictions Only six pregnancies examined in treatment group and males also chronically treated with ethanol such that the quality of the study is reduced.
Reference	Klassen, R.W. & Persaud, T.V.N. (1976) Experimental studies on the influence of male alcoholism on pregnancy and progeny. Exp. Pathol. 12, 38 - 45.
12.11.2004	(254)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Dominant lethal assay
Species	rat
Sex	male

Strain	Long-Evans
Route of admin.	drinking water
Exposure period	60 day
Doses	20% v/v ethanol solution given to 10 rats
Result	positive
Method	other
Year	1982
GLP	no data
Test substance	ethanol (64-17-5)
Method	Age at Study start: Not stated. Animals 200-300 g and were acclimated for 2 wk before mating. No of animals/group: 10. Dosage: Level of alcohol in the drinking water equivalent to a daily dose of 15.7 g/kg body weight. Vehicle: Distilled water. Duration of Test: Males treated for 60 days then mated with 3 females over three weeks. Frequency of treatment: Ad libitum for 60 days. Sampling: Testicular tissue examined after the third mating. Uterine contents examined on gestation day 20. Controls: Untreated males. Clinical observations: male bodyweights before and after 60 day exposure and at sacrifice. Histopathology: Testicular tissue. Criteria for evaluation: Dominant lethal index calculated as 100%x(1-litter size in treated group/litter size in control group). Criteria for selection of MTD: Not discussed.
Remark	Diluted to 20% v/v in distilled water.
Result	Both the number of resorptions and the percentage of litters with resorptions were increased. The index of dominant lethal mutations declined from 16.4 to 7.8 over three successive matings. Absolute and bodyweight relative testicular weights were decreased by ethanol treatment (20%) and seminiferous tubule diameters were decreased together with an increase in the number containing cellular debris. Mortality at each dose: None. Mutations etc. Not relevant. Clinical signs: No adverse signs were observed. Body weights: Male bodyweights were unaffected by ethanol treatment. Food/water consumption: Not presented.
Test Substance	Test substance was USP alcohol, 200 proof.
Reliability	(2) valid with restrictions
Reference	Mankes, R.F., leFevre, R.t Benitz, K.-F., Rosenblum, I. et al.

	(1982). Paternal effects of ethanol in the long Evans rat. J. Toxicol. Envir. Hlth 10:871-878.
12.11.2004	(255)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Dominant lethal assay
Species	rat
Sex	male
Strain	Wistar
Route of admin.	drinking water
Exposure period	up to 35 days
Doses	up to 30% alcohol in the drinking water given to an unspecified number of rats
Result	negative
Method	other
Year	1980
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Age at start of treatment: 6-7 weeks. TreatmentThree groups of rats (numbers unspecified) were treated as follows: group I, 30% ethanol for 4 days; group II, 15% ethanol for 5 days, then 20% for 30 days; group III, 15% for 5 days, 20% for a further 5 days, 25% for 10 days and then 30% ethanol for the final 15 days. One control group was untreated, while a positive control group was exposed to x-rays (200 R) prior to mating. After treatment, each male was paired with 2-3 females per week for 8 consecutive weeks. The females were killed 10 -11 days after removal from the males and examined for live and dead implantations. Investigations: Dead implantations, reduction of live implantations and total implantations were enumerated.
Result	There were no significant differences in the numbers of dead, live and total implantations at the pre-or postimplantation levels in the control (untreated) or ethanolic groups. In the positive control group there was a high incidence of dead implants and a reduction in the number of live implants. The pregnancy rate was lower in group II, but this was not thought to be treatment-related, as the effect was not seen at 30%.
Reliability	(2) valid with restrictions
Reference	Chauhan, P.S., Aravindakshan, M.. Kumar, N.S., Sundaram, K. (1980). Failure of ethanol to induce dominant lethal mutations in Wistar male rats. Mutation Res. 79: 263-275.

12.11.2004 (256)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Dominant lethal assay
Species	mouse
Sex	female
Strain	no data
Route of admin.	oral
Exposure period	unspecified
Doses	single dose 5 ml/kg body weight given to 31 mice
Result	negative
Method	other
Year	1975
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Females in pro-oestrus given a single dose of ethanol and mated on same day (2 females to 1 male). Pregnant females then dissected. Control group of 33 mice. Route of administration: presumably gavage.
Result	Ethanol produced no dominant lethal effects at a daily dosage of 5 ml/kg p.o.
Reliability	(4) not assignable
Reference	Machemer, L., Lorke, D. (1975). Experiences with the dominant lethal test in female mice. Effects of alkylating agents and artificial sweeteners on pre-ovulatory oocyte stages. Mutation Res. 29; 209-214.

12.11.2004 (257)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Dominant lethal assay
Species	mouse
Sex	female
Strain	C3H
Route of admin.	gavage
Exposure period	
Doses	single dose 1, 1.5 or 2 hr after mating 1 ml of 12.5% ethanol or distilled water
Result	
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)

Remark	Age at study start:10-12 weeks. Strain: { C3H x C58BL)F1 No. animals/dose: 47 ethanol treated vs. 43 controls mated at 1 hr; 24 ethanol treated vs. 24 controls mated at 1.5 hr; Three further experiments involved mating 1 hr (29 vs. 25 controls) or 2 hours (118 vs. 110) after ethanol treatment, with uterine analysis. Vehicle: Distilled water. Duration of test: 17 days investigations: Number of implantations per pregnant female, number of living embryos per pregnant female and % dead implants. Sampling: Eggs taken and examined microscopically; first-cleavage embryos taken for chomosome analysis. Clinical observations: None. Organs examined at necropsy: None.
Result	Treatment with ethanol at 1 or 1.5 hr after mating did not affect the number of implantations per pregnant female, the number of living embryos per pregnant female and the % dead implants. However, the pooled data (118 ethanol-treated vs. 110 controls) for rats treated at 2 hr post mating showed a significant increase in late (post 11 days) deaths (P = 0.002). Ethanol treatment was associated with a higher number of abnormal cells (P=0.039), i.e. trisomy possibly the result of clastogenicity or lagging of chromosomes in M-II.
Reliability	(4) not assignable
Reference	Washington, W.J., Cain, K.T., Cacheiro, N.L.A., Generoso, W.M. (1985). Ethanol-induced late fetal death in mice exposed around the time offertilization. Mutat. Res. 1985; 147: 205-210.
12.11.2004	(258)

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Test substance:	1-butanol
Test species/strain:	Mouse/NMRI (male and female)
Test method:	OECD No. 474 (Proposal for updating, ENV/EPOC (96)4) EPA/TSCA 789.5395 (August 1997) EEC Directive 92/69, B 12 (December 1992)
GLP:	Yes
Test results:	Oral gavage dose of 500, 1,000 or 2,000 mg/kg of n-butanol did not have any chromosome-damaging (clastogenic) effect, and there were no indications of any impairment of chromosome distribution in the course of mitosis at either the 24 or 48 hour time points.
Lowest dose producing	

toxicity: 2000 mg/kg
Effect on Mitotic Index or P/N Ratio: None
Genotoxic effects: + ? -
[ ] [ ] [X]
Comments: Both of the positive control chemicals, i.e. cyclophosphamide for clastogenicity and vincristine for spindle poison effects, led to the expected increase in the rate of polychromatic erythrocytes containing small or large micronuclei.
Reference: Engelhardt, D., and Hoffmann, H.D. Cytogenetic Study In Vivo with n-butanol in the Mouse Micronucleus Test - Single Oral Administration. (1998) Project No. 26M0346/974126, Department of Toxicology, BASF Aktiengesellschaft, D-67056. Ludwigshafen/Rhein, FRG.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Test substance: >95% 1-hexanol (111-27-3)

Remark: In common with other members of the aliphatic alcohols category 1-hexanol contains no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the range of category members including 1-hexanol are negative. Results from in vivo studies with other category members and/or supporting substances provide evidence that these alcohols are not genotoxic in vivo.

Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].
Conclusion: Not expected to be genotoxic in vivo.
Reliability: (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vivo is based are either guideline studies or publications with sufficient detail for assessment.
Reference: IPCS/WHO 1993 Toxicological evaluation of certain food additives and contaminants. 2-ethyl hexanol WHO Food Additives Series 32 pp 35-55.

SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic

Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

SIDS Dossier -Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G., Webb, C. 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium
12-SEP-2005 (28) (66) (67) (74)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Remark: In common with other members of the aliphatic alcohols category C6-12 alcohols (Types A,B,C and D) contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the range of category members (linear and essentially linear), including a negative Ames test for 1-octanol, are negative. Results from in vivo studies with other category members and/or supporting substances provide evidence that these alcohols are not genotoxic in vivo.

Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

Test substance: > 90% 1-octanol (111-87-5)

Conclusion: Not expected to be genotoxic in vivo.

Reliability: (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vivo is based are either guideline studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category
14-SEP-2005 (104) (105) (119)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Remark: The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5-C24-34) are negative including a study for 1-decanol [Ames].

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

Test substance: > 90% 1-decanol (112-30-1)
Conclusion: Not expected to be genotoxic in vivo.
Reliability: (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vivo is based are either comparable to or guideline studies or publications with sufficient detail for assessment.
Reference: IPCS/WHO 1993 Toxicological evaluation of certain food additives and contaminants. 2-ethyl hexanol WHO Food Additives Series 32 pp 35-55.

SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

SIDS Dossier - Octadecanol, 1995 with additional robust

summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category
12-SEP-2005 (51) (84) (85) (97)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	other: albino mice, CFW 1
Route of admin.	:	gavage
Exposure period	:	24, 48, 72 hours
Doses	:	5000 mg/kg bw
Result	:	negative
Method	:	OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year	:	1992
GLP	:	yes
Test substance	:	dodecanol (112-53-8)
Test substance	:	Tradename Lorol 12
Test condition	:	TEST ORGANISMS: Mouse CFW 1 - Age: 7-8 weeks - Weight at study initiation: males 21-27g, females 21-26g - No. of animals per dose: 6M + 6F ADMINISTRATION: - Vehicle: Arachis oil. - Duration of test: 1 day, single administration. - Frequency of treatment: Once. - Sampling times and number of samples: 24, 48 and 72 hours after treatment. Two slides were prepared for each animal and 1000 polychromatic erythrocytes (PCE) scored. - Control groups and treatment: Solvent control arachis oil, 10 ml/kg: positive control cyclophosphamide, 20 mg/kg; test substance 1-dodecanol 5000 mg/kg (dose volume 10 ml/kg) EXAMINATIONS: - Clinical observations: Daily - Organs examined at necropsy: None.

- Criteria for evaluating results: A statistically significant ($p<0.05$) increase in PCE compared to controls. Method used Kastenbaum & Bowman.
- Criteria for selection of M.T.D.: Based on a screening test. Effects seen at 5000 mg/kg were piloerection only.

Result : MORTALITY: None

CLINICAL SIGNS: Piloerection in all test animals.

NECROPSY FINDINGS: Not reported.

BODY WEIGHT CHANGES: Not reported.

FOOD AND WATER CONSUMPTION CHANGES: Not reported.

PCE/NCE RATIO: There was no effect on this ratio.

GENOTOXIC EFFECTS: There was no increase in the incidence of micronucleated cells in the test group. The incidence of micronuclei in the contorl group was within historical control ranges. The positive control group produced an appropriate increase in numbers of micronucleated cells.

STATISTICAL RESULTS: No statistically significant increase in micronucleated polychromatic erythrocytes compared to vehicle controls, the positive control group did produce a statistically significant increase.

Conclusion : Lorol 12 did not increase the % of micronucleated erythrocytes or the PCE:NCE ratio in mice at any time interval after treatment (24, 48 or 72 hours) at dose levels up to 5000 mg/kg bw when compared to vehicle controls.

Reliability : (1) valid without restriction
Guideline study

Source : Banduhn, 1992
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Banduhn, N. 1992. 1-Dodecanol: Micronucleus test in vivo on bone marrow cells of the mouse. Henkel KGaA Report No. 920162.

11.08.2005 (3)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)</u>

Remark: The category members contain no structural elements which may

be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-octanol and 1-decanol, dodecanol, tetradecanol and hexadecanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

Source: Hayes Consultancy Service Bromley, Kent
Test substance: > 95% 1-Tetradecanol (112-72-1)
Conclusion: Not expected to be genotoxic in vivo.
Reliability: (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
Reference: IPCS/WHO 1993 Toxicological evaluation of certain food additives and contaminants. 2-ethyl hexanol WHO Food Additives Series 32 pp 35-55.

SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category
15-SEP-2005 (43) (66) (67) (78)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Remark: The category members contain no structural elements which may

be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, hexadecanol and octadecanol [Ames] are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

Test substance: >= 95% 1-hexadecanol (36653-82-4)

Conclusion: Not expected to be genotoxic in vivo.

Reliability: (2) valid with restrictions

The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

15-SEP-2005 (80) (81) (94)

<u>1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)</u>

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male
Strain	:	other: ddY

Route of admin.	:	gavage
Exposure period	:	24 hours
Doses	:	360, 730, 1450 mg/kg (single dose) or 730 mg/kg (adminstered 4 times in 24 hours)
Result	:	negative
Method	:	other: mouse bone marrow micronucleus test to protocol to the Japanese Labour Ministry
Year	:	1982
GLP	:	no data
Test substance	:	octadecanol (112-92-5)
Test substance	:	Octadecanol (112-92-5) (Kalcohol 80, 718)
Test condition	:	TEST ORGANISMS: Mice - Age: 6 weeks - Weight at study initiation: not reported - No. of animals per dose: Groups of 5 or 6 ADMINISTRATION: Gavage - Vehicle: Olive oil, dosing volume 25 ml/kg - Duration of test: 1 or 4 doses. - Frequency of treatment: Once or 4 times in 24 hours. - Sampling times and number of samples: 24 hours after a single does, 5 days after the first administraton of the repeated doses. 2000 red blood cells scored per smear for micronuclei, 1000 scored for reticulocytes. - Control groups and treatment: Stearyl alcohol single oral doses of 0.36, 0.73 or 1.45 g/kg/day or 4 doses of 0.73 g/kg/day in a 24 hour period. Positive control mitomycin C 3 mg/kg intraperitoneally. Solvent control olive oil 25 ml/kg EXAMINATIONS: - Clinical observations: Not reported - Organs examined at necropsy: Not reported - Criteria for evaluating results: Not reported - Criteria for selection of M.T.D.: The maximum single dose was half the LD50. Repeated doses were 1/4 LD50. STATISTICAL ANALYSIS: Kastenbaum & Bowman
Result	:	MORTALITY: Not reported CLINICAL SIGNS: Not reported NECROPSY FINDINGS: Not reported

BODY WEIGHT CHANGES: Not reported

FOOD AND WATER CONSUMPTION CHANGES: Not reported

EFFECT ON MITOTIC INDEX OR PCE/NCE RATIO: There were no effects on the incidence of reticulocytes following a single dose of stearyl alcohol. Repeated exposure showed a decrease [controls 61.3%; treated 52.9%]

GENOTOXIC EFFECTS: No significant increase increase in numbers (%) of micronucleated erythrocytes. 10000 - 12000 observed.

NOAEL (NOEL) (C) / LOAEL (LOEL) (C): A single dose of 1450 mg/kg/day or a total repeated dose of 2920 mg/kg did not increase the incidence of micronuclei. There was no reported assessment of effects on the live animals.

Conclusion : Stearyl alcohol (Kalcohl 80, 718) did not increase the incidence of micronucleated cells in mouse bone marrow erythrocytes following a single oral dose level up to and including 1450 mg/kg or a total of 2920 mg/kg adminstered as 4 doses in a 24 hour period.

Reliability : (2) valid with restrictions
Limited documentation but acceptable for assessment

Source : Hachiya et al, 1982
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference

Hachiya, N.; Takeya, A.; Takizawa, Y. 1982. Japanese J. Public Health 29(5): 236-239, 1982 (In Japanese, translation available).

SIDS Dossier on 1-Octadecanol. 1993b. Environmental Protection Agency, Denmark. 6 June 1993.

12.08.2005 (8) (23)

<u>1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)</u>

Remark: The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34), including data for hexadecanol, octadecanol and docosanol, are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic

in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

Test substance: >= 90% 1-eicosanol (629-96-9)

Conclusion: Not expected to be genotoxic in vivo.

Reliability: (2) valid with restrictions

The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

15-SEP-2005 (18) (23)

<u>1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)</u>

Type: Micronucleus assay

Species: mouse **Sex:** male/female

Strain: NMRI

Route of admin.: gavage

Exposure period: Single dose

Doses: 50, 150 500 mg/kg bw

Result: negative

Method: other: similar to OECD 474

Year: 2002

GLP: yes

Test substance: >95% 1-docosanol (661-19-8)

Result: MORTALITY: One male and one female mouse died either spontaneously or due to gavage error.

CLINICAL SIGNS: Not reported

NECROPSY FINDINGS: Not reported.

BODY WEIGHT CHANGES: Not reported.

FOOD AND WATER CONSUMPTION CHANGES: Not reported.

EFFECT ON PCE/NCE RATIO: No increase in the ratio.
No increase in the % of micronucleated erythrocytes.

GENOTOXIC EFFECTS: None for behenyl alcohol, the positive controls showed an appropriate response.

STATISTICAL RESULTS: No statistical significance.

Source: Iglesias, 2002a

Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS:
- Age: At least 10 weeks
- Weight at study initiation: Not reported.
- No. of animals per dose: 6 males + 6 females

ADMINISTRATION:
- Vehicle: polyethylene glycol (PEG)
- Duration of test:
- Frequency of treatment: A single oral dose was administered.
- Sampling times and number of samples: 24, 48 or 72 hour harvest. At least one slide per sample (no other details given). For each animal 1000 PCE's were scored for micronuclei.
- Control groups and treatment: Vehicle control (PEG), 30, 150 and 500 mg/kg Behenyl alcohol at a volume of 10 ml/kg bw. Positive control cyclophosphamide 40 mg/kg.

EXAMINATIONS:
- Clinical observations: Not reported
- Organs examined at necropsy: Not reported
- Criteria for evaluating results: A statistically significant dose-related increase in numbers of micronucleated polychromatic erythrocytes or a reproducible statistically significant positive response for at leats on of the test points. Statistical analysis used the Mann-Whitney test, significance at $p<0.05$.
- Criteria for selection of M.T.D.: 500 mg/kg/day was considered to be the maximum tolerated dose based on a previously conducted experiment however the criteria were reported.

Test substance: C22 alcohol [behenyl alcohol] CAS RN 661-19-8

Conclusion: Behenyl alcohol (C22) did not increase the % of micronucleated erythrocytes or the PCE:NCE ratio in mice at any time interval after treatment (24, 48 or 72 hours) at dose levels up to 500 mg/kg bw when compared to vehicle controls.

Reliability: (2) valid with restrictions
Comparable t guideline studye with acceptable restrictions. Similar to OECD 474 but full experimental details were not reported in the publication. In particular there were no details of toxicity to the mice although the top dose was reported as the MTD.
Flag: Critical study for SIDS endpoint
Reference: Iglesias, G, JJ Hlywka, JE Berg, MH Khalil, LE Pope and D Tamarkin. 2002a. The toxicity of behenyl alcohol: I. Genotoxicity and subchronic toxicity in rats and dogs. Regulatory Tox. and Pharm. 36, 69-79.
06-AUG-2005 (15)

1-Tetracosanol, 1-Hexacosanol, 1-Octacosanol, and 1-Triacontanol for their respective Aluminum Salts

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	NMRI
Route of admin.	:	gavage
Exposure period	:	5 days
Doses	:	2000 mg/kg/day
Result	:	negative
Method	:	other: similar to OECD 474
Year	:	1998
GLP	:	no data
Test substance	:	C24-C34 alcohols
Test condition	:	TEST ORGANISMS: mouse NMRI - Age: 40 days - Weight at study initiation: 18-22 g - No. of animals per dose: 6 male + 6 female ADMINISTRATION: gavage - Vehicle: suspension of gum arabic in water 10 mg gum arabic/kg - Duration of test: 5 days - Frequency of treatment: daily - Sampling times and number of samples: Single sampling of bone marrow (ex femur) 24 hours after final dose. _ Cells evaluated: 2000 - Control groups and treatment: vehicle control same treatment regime as the treated group, positive control cyclophosphamide single intraperitoneal dose of 50 mg/kg. Treated and vehicle controls received a constant dose volume of 1 ml/kg.

EXAMINATIONS:
- Clinical observations: Not reported
- Organs examined at necropsy: None
- Criteria for evaluating results: Total number of micronuclei, %PCE and PCE/NCE ratio.
- Criteria for selection of M.T.D.: Based on previous toxicity testing in this species the limit dose of 2000 mg/kg was used.

STATISTICAL ANALYSIS:
Increase in %PCE in total erythrocyte population evaluated using Mann Whitney U test, Comparision of PCE/NCE index between groups using Kruskall Wallis.

Result : MORTALITY: None

CLINICAL SIGNS: None reported

NECROPSY FINDINGS: None reported

BODY WEIGHT CHANGES: None reported

FOOD AND WATER CONSUMPTION CHANGES: Not reported

EFFECT ON PCE/NCE RATIO: No difference between treated and vehicle control groups significant reduction in positive controls.

PCE/NCE (determinations in 2000 erythrocytes/animal)
Vehicle control Male: 1.116 +- 0.23 Female: 1.18 +- 0.15
Treated 2000 mg/kg Male: 2.33 +- 0.25 Female: 1.09 +- 0.09
Positive control Male: 0.72 +- 0.15* Female: 0.73 +- 0.11*

* significant p<0.05 U (Mann Whitney)

GENOTOXIC EFFECTS: None

Total micronuclei (determinations in 2000 PCE/animal)
Vehicle control Male: 21 Female: 25
Treated 2000 mg/kg Male: 28 Female: 22
Positive control Male: 435 Female: 391

MN/PCE (determinations in 2000 PCE/animal) x 10 to power 3
Vehicle control Male: 1.75 +- 1.04 Female: 2.08 +- 0.66
Treated 2000 mg/kg Male: 2.33 +- 0.41 Female: 1.09 +- 0.09
Positive control Male: 37.73 +- 7.47* Female: 31.75 +- 8.08*

* significant p<0.05 U (Mann Whitney)

NOAEL (NOEL) (C) / LOAEL (LOEL) (C): NOAEL 2000 mg/kg/day

mPCE FREQUENCY: No significant difference between treated and control groups.

STATISTICAL RESULTS: See above

Conclusion : The product D-002 did not increase the numbers of micronucleated cells in the bone marrow of mice following repeated oral administration of the limit dose of 2000 mg/kg/day for 5 days.

Reliability : (2) valid with restrictions
Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment. Although not conducted specifically to OECD regulatory guidelines, the methodology appeared similar. Results were reported for the group (no individual animal results were provided in the publication)

Flag : Critical study for SIDS endpoint

Reference Rodeiro, I. et al 1998 Estudio genotoxico del D-002, un producto con actividad antiulcerosa. (Genotoxic study of D-002, a product with antiulcerous activity) Rev. Toxicol. 15:117-121 [In Spanish, English translation available].

12.04.2005 (6)

1-Tetracosanol, 1-Hexacosanol, 1-Octacosanol, and 1-Triacontanol for their respective Aluminum Salts

Type : Dominant lethal assay
Species : mouse
Sex : male/female
Strain : NMRI
Route of admin. : gavage
Exposure period : 6 weeks females; 8 weeks males
Doses : 0, 25, 125 and 625 mg/kg/day
Result : negative
Method : other: similar to OECD 478
Year : 1998
GLP : no data
Test substance : C24-C34 alcohols

Test condition : TEST ORGANISMS: Mouse NMRI
- Age: 40 days
- Weight at study initiation: 18-20 g
- No. of animals per dose: 40 females/group; 25 males /group.

ADMINISTRATION: gavage
- Vehicle: suspension of gum arabic in water 10 mg gum arabic/kg
- Duration of test: 6 weeks for treated female groups, 8 weeks for males.
- Frequency of treatment: Daily
- Sampling times and number of samples:
- Control groups and treatment: vehicle control adminstered orally as for treated groups, 5 days intraperitoneally for positive control (cyclophosphamide 50 mg/kg) and control with saline.

EXAMINATIONS: At the end of the treatment period females were mated over a period of 1 week, 2 females to 1 untreated male. Treated males were mated with 2 females per male at two successive intervals each mating period being for one week to ensure that the effect of the drug was evaluated at 2 stages of spermatogenesis. The females from both studies were sacrificed 17-19 days after the first day of mating.
- Clinical observations: Mortality and body weight (recorded weekly)
- Organs examined at necropsy: uterus and ovaries
- Criteria for evaluating results: Number of implantations, late and early resorptions, % pregcant females, corpora lutea and numbers of live foetuses were examined.
- Criteria for selection of M.T.D.: A single oral dose produced no adverse effects at 5 g/kg/day. The study was designed to detect the cumulative effects of D-002.

STATISTICAL EVALUATION: Krusakall Wallis (non-parametric analysis of variance) for all parameters except frequency of mortality/pregnant female which used the Fischer Exact Probability test.

Result : MORTALITY: None

CLINICAL SIGNS: Not reported

NECROPSY FINDINGS: Not reported

BODY WEIGHT CHANGES: Not reported

FOOD AND WATER CONSUMPTION CHANGES: Not carried out

NOAEL: 625 mg/kg/day over a 6 week period for females or an 8 week period for males.

TEST PARAMETERS: Treated females n= 30-37
% Pregnant females/Implantations/Corpora lutea/Live foetuses/Early

resorptions/Late resorptions per female/group
Vehicle control: 38/10.2/10.6/9.5/21 of 33/2 of 33
25 mg/kg 85/9.7/10.1/9.0/22 of 34/2 of 34
125 mg/kg 75/10.7/10.9/10.3/8 of 30/3 of 30
625 mg/kg 88/9.7/10.0/9.1/18 of 35/1 of 35
Saline control 91/11.1/12.3/10.5/15 of 36/5 of 36
Positive control 92/8.3*/12.2/4.7*/60 of 37**/52 of 37**

* p<0.05 Kruskall Wallis ** p<0.05 Fischer exact

Females (n =44-48) mated with treated males.
1st week of mating
% Pregnant females/Implantations/Corpora lutea/Live foetuses/Early resorptions/Late resorptions per female/group
Vehicle control: 92/12.8/13.8/12.1/ 25 of 46/ 5 of 46
25 mg/kg: 88/11.4/12.8/10.7/ 32 of 44/ 2 of 44
125 mg/kg: 94/11.8/13.4/11.1/ 31 of 47/ 2 of 47
625 mg/kg: 94/12.0/13.1/11.5/ 19 of 47/ 2 of 47
saline control: 95/11.1/12.5/10.3/ 23 of 48/ 2 of 48
positive control: 83/7.7*/11.3/4.2*/ 87 of 46**/ 62 of 46**

* p<0.05 Kruskall Wallis ** p<0.05 Fischer exact

Results for the second week of mating followed a similar pattern to those reported above.

STATISTICAL RESULTS: See above

Conclusion : There is no evidence of dominant lethality in the mouse following repeated oral exposure to D-002 at dose levels up to 625 mg/kg/day for 6 weeks in females and 8 weeks in males as indicated by early and late resorptions, foetal survival, numbers of corpora lutea and numbers of implantations/female/group.

Reliability : (2) valid with restrictions
Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment. Although not conducted specifically to OECD regulatory guidelines, the methodology appeared similar. Results were reported for the group (no individual animal results were provided in the publication)

Flag : Critical study for SIDS endpoint

Reference Rodeiro, I. et al 1998 Estudio genotoxico del D-002, un producto con actividad antiulcerosa. (Genotoxic study of D-002, a product with antiulcerous activity) Rev. Toxicol. 15:117-121 [In Spanish, English translation available].

12.04.2005 (6)

5.8.1 Toxicity to Fertility

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	Two generation study
Species	Mouse
Sex	male/female
Strain	CD-1
Route of admin.	drinking water
Exposure period	105 weeks
Frequency of treatm.	ad libitum
Premating exposure period	
Male	Parental 7 days; Ft 74 days
Female	Parental 7 days; Ft 74 days
Duration of test	
No. of generation studies	2
Doses	5, 10 and 15% v/v in water
Control group	yes, concurrent no treatment
NOAEL parental	= 15%
NOAEL F1 offspring	= 10%
NOAEL F2 offspring	< 15%
Result	No observed effect on fertility
Method	other: NTP protocol
Year	1985
GLP	no data
Test substance	other TS: 92% ethanol (64-17-5)

Method

Age at onset: P animals 6 weeks at receipt, 11 weeks at first exposure. No. of animals per sex per group: 20 also 20 F1 animals at the high dose mated at 74 days old.
Ethanol administered in deionized, filtered water.
P generation dosed for 7 days pre-mating and then for 98 days.
F1 animals continued on dosing until mating.

Animals mated in cohabiting pairs; litters were proof of pregnancy.

Litters were not standardized.
Clinical signs, oestrous length etc. were not evaluated.
Epididymal and vas sperm were evaluated for concentration, motility and morphology in F1 males only.
High dose F1 animals had liver, kidney/adrenal and male sex organs weighed at termination.
F2 data were for litter sizes etc. Only.

Result

Parental F1 data: Ethanol treatment had no effect on

bodyweights and on the proportion of breeding pairs producing at least 1 litter during the continuous breeding phase or the number of litters per pair. Fertility indices were 97,100,100 and 94% in the controls and 5%, 10%,15% ethanol groups respectively.

Offspring data: F1 offspring of the 15% ethanol pairs had fewer live pups per litter. their F2 offspring weighed less as pups than control pups, males, females or both sexes. Fertility indices in F1 matings were 85% and 85% in the controls and 15% ethanol groups respectively. Other reproductive performance indices e.g. gestation index, changes in lactation and changes in oestrous cycles were not studied

Effects on sperm and male reproductive organs: In the F1, 15% ethanol group there was a significantly decreased %motile sperm but no changes in sperm concentration, %abnormal sperm or %tailless sperm. There was a significant decrease in testis, epididymis and seminal vesicle weight

Gestation index, changes in lactation and changes in oestrus cycles were not studied.

Haematological, clinical biochemical, gross pathological and histopathological changes were not studied.

Mortality in P animals is reported but not discussed. F1 males from the 15% group at adulthood had decreased bodyweight and and decreased weight of testis and epididymides and seminal vesicles. In F2 females, relative liver and kidney/adrenal weights were increased.

Offspring toxicity:
Litter size and weights: Not given.
Sex ratios: Not influenced by treatment Viability index: Not reported. Litters born to P at 15% ethanol had reduced number of live pups per litter.
Post natal survival until weaning: Not reported.
Posta natal growth: Pups born in final F1 generation of animals exposed to 15% ethanol pre- and post-natally weighed less than controls at birth and days 21 and 74.
Vaginal opening or preputial separation: Not studied.
Anogenital distance: Not measured.
Organ weights: Described above.
Gross pathology: Not examined.

Conclusion Overall, ethanol in drinking water at concentrations up to 15%

	(equivalent to 20.7 g/kg/day) had no demonstrable effect on fertility in this two generation study.
Reliability	(1) valid without restriction Well reported study but not to a standard protocol. Very high doses used and no NOAEL identified for all endpoints.
Flag	Critical study for SIDS endpoint
Reference	George, J., Myers, C., Reel, J. et al. (1985). Ethanol: Reproduction and fertility assessments in CD-2 mice when administered in the drinking water. NTP PB86144979.
12.11.2004	(283)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	One generation study
Species	Mouse
Sex	Male
Strain	Swiss Webster
Route of admin.	oral feed
Exposure period	49 days
Frequency of treatm.	ad libitum
Premating exposure period	
Male	Sequential matings through 7 weeks of exposure
Female	None
Duration of test	7 weeks
No. of generation studies	1
Doses	10% and 25% of ethanol-derived calories
Control group	Yes
NOAEL parental	= 10 %
NOAEL F1 offspring	= 25%
NOAEL F2 offspring	
Result	Fertility not affected
Method	other
Year	1989
GLP	no data
Test substance	ethanol (64-17-5)
Method	Number/age of animals: 20 males per group, 75 days old at start of treatment. Vehicle etc: Ethanol providing 10 or 20% of calories in a nutritionally balanced liquid diet. Two control groups consisting diets compensated or not for ethanol calories. Dosing schedules: Males were given ethanol or control treatments for 7 weeks prior to mating with untreated females. Mating procedure: 2 females per male for 4 hours; vaginal plugs were treated as evidence of pregnancy. Females were allowed to give birth and offspring were counted, weighed, culled and re-

weighed at 21 days. Litters were standardized by culling at birth to 8 per dam.

Parameters assessed: Vital and functional observations were maintained on P and F1 generations.

Result

Sperm quality, anogenital distance and organs at necropsy were not evaluated.
Parental data Bodyweight: Paternal bodyweights were less at 25% ethanol-derived calories than at 10 or 0%. Offspring bodyweights were not affected by treatment.
Food/water consumption: High-dose males consumed less diet. (NB pair fed controls).
Clinical signs: None reported.
Fertility index: At least 80% for each ethanol concentration at each time point. Fertility was at least as great as in pair-fed controls.
Precoital interval: Not measured.
Duration of gestation: To term.
Gestation index: Not given.
Changes in lactation, oestrus cycles, sperm, haematology, clinical chemistry, gross pathology, no. of implantations, no. of corpora lutea, ovarian primordial follicle count, organ weight change and histopathology:
Not studied.
Mortality: Not reported.

Offspring toxicity:
No dose-related observations were made.
Litter sizes and weights: Not affeceted by paternal exposure.
Sex and sex ratios: Not affected by paternal, exposure.
Viability index: Not measured.
Post natal survival: No mortality reported.

Effects on offspring: Not studied.
Postnatal growth: Not affected by day 21.
Vaginal opening: Not studied.
Anogenital distance, organ weights and gross pathology: Not studied.

Result

No toxic responses were noted in treated males other than decreased bodyweight gain at 25% ethanol-derived calories in diet. Fertility over 7 weeks of treatment was not affected.

No adverse effects on offspring were noted as a function of either level of paternal ethanol treatment or duration of treatment.

	Fertility was at least as great as in pair-fed or standard controls.
Reliability	(2) valid with restrictions Well reported study but not to a standard protocol. Very high doses used.
Reference	Abel, E. (1989). Duration of paternal alcohol consumption does not influence offspring growth and development. Growth Devel. Aging 53: 195-199.
12.11.2004	(284)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	One generation study
Species	Rat
Sex	Female
Strain	other: Holtzmann
Route of admin.	oral feed
Exposure period	8 or 16 weeks before mating
Frequency of treatm.	ad libitum daily
Premating exposure period	
Male	no treatment
Female	3 or 6 weeks
Duration of test	
No. of generation studies	
Doses	5% in liquid feed
Control group	Yes
NOAEL parental	< 5%
NOAEL F1 offspring	<= 5%
NOAEL F2 offspring	
Result	Fertility not affected although oestrous cycle length was prolonged and irregular
Method	other
Year	1982
GLP	no data
Test substance	ethanol (64-17-5)

Method	No, and age of animals: 10 per group, age 20 days. No F2 generation. Ethanol was supplied in a liquid diet for 16 weeks prior to mating or for 8 weeks followed by 8 weeks on standard diet. Dosing ended after mating. Two Control groups were used, one receiving standard diet the other pair fed with 5% ethanol in diet. Mating procedure was by 1:1 cohabitation with a fertile male for 14 hr. proof of pregnancy was a sperm-positive vaginal smear. Study

ended with delivery of F1 pups.
Oestrous cycle length and pattern was recorded.
Growth performance in Ft pups was followed.
Statistical test was one-way ANOVA.

Result

Parental data:
Effect of duration of exposure, not dose, was assessed.
Administration of 5% for 16 weeks, not 8 weeks, increased oestrus cycle length and irregularity. Age to vaginal patency was increased by both regimen. No abnormalities of ovaries or uteri were found.
Bodyweight: Maternal bodyweights were measured but not reported.
Offspring bodyweights were not affected by treatment.
Food/water consumption: Not reported but must have been recorded.
Clinical signs: None reported.

Fertility index: At least 80% far each ethanol concentration at each time paint. Fertility was at least as great as in pair-fed controls.
Precoital interval: Not measured.
Duration of gestation: Not reported.
Gestation index: All females delivered live litters.
Changes in lactation, oestrus cycles, sperm, haematalogy, clinical chemistry, grass pathology, no. of implantations, no. of corpora lutea, ovarian primordial follicle count, and organ weight change: Not studied.
Histopathology: All ovaries and uteri examined were normal.
Mortality: None reported.

Offspring taxi city:
No. dose-related observations were made.
Litter sizes and weights: Not affected by maternal exposure.
Sex and sex ratios: Not given.
Viability index: Not measured.
Past natal survival: No. mortality reported.
Effects an offspring: Not studied.

Result

Postnatal growth: Not studied.
Vaginal opening: Average age of vaginal potency was 72-77 days in bath groups and significantly older than in control groups (41-58 days).
Anogenital distance, organ weights and grass pathology: Not studied.
No. adverse effect an fertility, litter size or neonatal bodyweight was detected. Irregular cycles and longer oestrous cycles were noted in rats fed for 16 weeks but not after 8 weeks with 8

	weeks recovery period. Average age of vaginal potency was 72-77 days in both groups of ethanol treated rats versus 41-58 days in controls.
Reliability	(2) valid with restrictions Well reported study but not to a standard protocol. Very high doses used and no NOAEL identified.
Reference	Krueger, WA, Bo, W.J., Rudeen, PK Female reproduction during chronic ethanol consumption in rats. Pharmacol. Biochem. Behav. 1982; 17: 629-631.
12.11.2004	(285)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	One generation study
Species	Rat
Sex	Female
Strain	other: Holtzmann
Route of admin.	oral feed
Exposure period	55 days
Frequency of treatm.	ad libitum daily
Premating exposure period	
Male	None
Female	50-55 days
Duration of test	
No. of generation studies	
Doses	2.5% and 5% in feed, estimated 8-12 g/kg/day and 12-14 g/kg/day
Control group	no data specified
NOAEL parental	= 2%
NOAEL F1 offspring	
NOAEL F2 offspring	
Result	Ovarian function was suppressed at the high dose
Method	other
Year	1982
GLP	no data
Test substance	ethanol (64-17-5)
Method	No. and age of animals: 8-11 per group aged 20 days at start. Vehicle etc: Ethanol was supplied in a liquid diet. Dosing schedule; Pair-fed controls were used at each dose for P animals with ethanol in diet ad lib for 50-55 days. No matings attempted so no F1 and F2 animals. Litter standardization: Not applicable.

	Animals were weighed weekly and examined daily far vaginal patency. Once patent, vaginal lavages were made daily. Oestrous cycle length and pattern: - length but not pattern determined. Sperm examination: Not applicable. F1 and F2 observations: Not applicable.
Remark	This study was to assess ovarian function as a possible factor in fertility studies following ethanol exposure. It is an adjunct to a study by the same authors demonstrating absence of effect an fertility but evidence of disturbed ovarian function. Parental and offspring data are not applicable in this study.
Result	Ovarian function was supressed in rats that achieved blood alcohol levels of 250 mg/100 ml. Animals receiving 5% ethanol (but not 2.5%) in liquid diet had longer time to vaginal patency, failed to. begin oestrus cycles, showed decreased bodyweight gain, had ovaries containing only a single generation of corporea lutea, had infantile vaginal and uterine epithelium and decreased uterine and ovarian weight.
Reliability	(2) valid with restrictions Well reported study but not to a standard protocol. Very high doses used.
Reference	Bo, E.J., Krueger, WA, Rudeen, P.K., Symmes, SK Ethanol-induced alterations in the morphology and function of the rat ovary. Anat. Rec. 1982; 202: 235-260.
12.11.2004	(286)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	One generation study
Species	Rat
Sex	Female
Strain	Wistar
Route of admin.	oral feed
Exposure period	49 days (animal age 28-77 days)
Frequency of treatm.	Daily
Doses	5% in feed, estimated 12,000 to 14,000 mg/kg/day
Control group	other: See method details
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Method	Number of animals: 100, ex Charles River Breeding Labs,

individually caged.
Ethanol fed animals received a liquid diet with ethanol accounting for 35% of total calories. Pair fed isocaloric controls (using dextrimaltose as alternative to ethanol.) Controls: ad libitum intact and ad libitum oophorectomized (Feed: Lab Blox F4 ex Best Feeds, Oakdale, Pa) Gross and microscopic anatomy: Animals sacrificed by exsanguination, 67 mls of blood kept for analysis. Liver, ovaries, uterus and fallopian tubes removed and weighed, preserved in Bouin's solution. Histological sections stained with hematoxylin and eosin. Liver assessed for degree of fat, necrosis and inflammation. Ovaries assessed for corpus lutea, corpus hemorrhagica, and numbers/development of Graafian follicles.
Uterus/fallopian tubes assessed for thickness of endometrium, type of and secretory activity of the epithelial lining cells and thickness of the muscle wall of each organ. Cervix/vagina examined for thickness of epithelial cell lining and signs of estrogen stimulation.
Plasma steroids and gonadotropins. All assessed by radioimmunoassaywith following levels of detection: Progesterone 10pg, Estradiol 0.1 pg, estrone 0.2pg, corticosterone 20pg, gonadotropin 4ng/ml. All measurements in duplicate.
liver: Enzyme function assessed by measuring serum alkaline phosphatase, gamma glutamyl transpeptidase, glutamic pyruvic and glutamic oxalacetic transaminase activities.
Blood ethanol: measured using blood samples obtained 1 day before sacrifice between 9-11 am and before feeding.
Statistical analysis: Student t test. "Probable significance" at p<O.05 and "significance" at p<O.01

Remark The reported blood ethanol level was relatively low (110±9 mg/dL) but the timing of the sample (taken 09.00 - 11.00 hours) was probably inappropriate to detect the peak likely at the usual time of feeding during the previous evening.

Result Growth (body weight at sacrifice): ethanol fed: 138 +1-5.3g; isocaloric controls: 161.6+/-3.8g. Significant difference (p<O. 01).
Anatomy: Livers of alcohol fed animals significantly larger than controls (p<0.01. Treated animals 10.6g+I-0.5, isocaloric controls 6.4g+I-0.3, ad libitum controls 8.3g+I-0.2). Ethanol treated animal livers markedly more fatty in appearance.
Ovaries: Marked weight loss in treated animals (30.6 +/- 2.2 mg versus 75.5 +/- 3.9 mg for isocaloric controls and 91.4 mg +/- 0.2 mg for ad libitum controls). Weight loss significant even when corrected for body weight. Reduction in ovarian mass due to absence of developing follicles, corpus lutea and corpus

hemorraghagica.
Histology: Differences in appearance of uterus, cervix and vagina between treated and untreated animals.
Uterus/fallopian tube: Marked weight loss in treated animals (39.0+/-4.1 mg versus 180.5+/-18.7 mg for isocaloric controls and 306 mg+/-15.5 mg for ad libitum controls). Weight loss significant even when corrected for body weight.

Plasma steroid and gonadotropin levels (n=25):
Plasma estradiol reduction seen in treated animals (ethanol fed: 27.5+/1.2pg/ml; isocaloric controls: 33.3+1-1.5 pg/ml; ad libitum intact controls:
48.0+/-1.4pglml; p<0.01). However no statistically significant reduction relative to oophorectomized control (29.8+1-1.6 pg/ml).
Plasma progesterone reduction seen (ethanol fed: 23.3+/-4.3 pg/ml;
isocaloric controls: 54.3+1-7.3 pg/ml; ad libitum intact controls: 41.7+/6.7 pg/ml; p<0.01). However no statistically significant reduction relative to oophorectomized control (18.0+1-0.6pg/ml).
Plasma estrone increase seen (ethanol fed: 156.0+/-26.7pg/ml; isocaloric controls: 114.9+/-13.9pg/ml; ad libitum intact controls: 80.5+/-6.3pg/ml;
p<0.01); oophorectomized control (48.0+/-5.2 pg/ml).
Plasma corticosterone levels increased (ethanol fed: 74.0+/-9.0ug/dl; ad libitum controls: 48.0+/-6.0 µg/dl; p<0.05). However no statistically significant reduction relative to pair fed controls (78.0+/- 9.0 µg/dl).
Plasma lutenizing hormone levels increased (ethanol fed: 68.7+/-5.7 ng/ml;
ad libitum controls: 43.5+/-7.0 ng/ml; p<O.01). However no statistically significant reduction relative to pair fed controls (79.4.0+/-6.8 ng/ml). All significantly less (p<O.01) than oophorectomized ad libitum control.
Plasma follicle stimulating hormone levels not statistically different but all significantly less (p<0.01) than oophorectomized ad libitum control.

Biochemical liver function:
Serum glutamic oxalo-acetic-acid-transaminase and serum glutamic pyruvic transaminase levels increased in treated animals (2.5x control levels). Alkaline phosphatase 50% greater in treated animals (all p<O.01).
Gamma glutamyl transpeptidase activity not detected in any controls but reproducibly measured (2.3 +/- IU/ml) in ethanol

	fed animals. Blood ethanol levels: 110 +/- 9.0 mg/1. Not detected in any controls.
Reliability	(2) valid with restrictions Well reported study but not to a standard protocol. Very high doses used and no LOAEL identified.
Reference	Van Thiel, D.H., Gavaler, J.S., Lester, R. Alcohol-induced ovarian failure in the rat. J. Clin. Invest. 1976; 61: 624-632.
12.11.2004	(287)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Fertility
Species	Rat
Sex	Male
Strain	Sprague-Dawley
Route of admin.	Gavage
Exposure period	9 weeks
Frequency of treatm.	twice per day
Premating exposure period	
Male	9 weeks
Female	
Duration of test	
No. of generation studies	
Doses	0, 2, 3 g/kg
Control group	other: concurrent vehicle and concurrent no treatment
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Method	Animals: Supplied by Charles River, 2 Months old at acquisition; acclimated for 2 weeks. Environment: 22 +/-1 degree C; relative humidity 45 +/- 5%; 12 hr: 12 hr light-dark cycle. Feed: Laboratory feed and water ad libitum. Treatment: After acclimation, groups of 20 male rats were intubated at 0900 and 1600 hrs with 3g/kg ethanol (15% w/v in distilled water), 2g/kg ethanol or vehicle (distilled water) only. Groups receiving 2 g/kg or 0 g/kg were paired fed with those receiving 3 g/kg and a fourth group received no gavage treatment. This continued for 9 weeks before breeding with 70 to 90-day-old females.

Controls: Distilled water by gavage (Group 3) or no gavage treatment (Group 4). Offspring of these groups were compared to. evaluate the potential for handling stress.
Evaluation of pups: After birth, pups were examined and weighed and litters were culled to 10 per female. Culled pups were subjected to brain and adrenal gland weight measurements. Offspring were weighed at 7, 14 and 21 days. At 7 days old, three males and 3 females from each of 6 litters were culled and their brain and adrenal gland weights determined.
At 21 days, this was repeated with inclusion of more organ weights. Blood alcohol levels were determined after breeding was determined at 1,2,3 & 5 hours after dosing.
Statistical analysis: ANOVA and Duncan's Multiple Range tests on parametric data; Chi-square on non-parametric data.

Remark

Paternal alcohol exposure did not influence litter size, average birth weight per pup or postnatal bodyweights in offspring. A study of runts suggested an influence of ethanol on individual sperm rather than on entire sperm production. The small but significant effect on male : female ratio (53 to 45%) was unexpected and is without explanation. An apparent effect on adrenal gland weight at birth is difficult to interpret, as this did not persist through offspring growth and development. An effect on spleen and heart weight indicates that paternal alcohol exposure may produce gross changes in offspring as well as functional changes.

Result

6 Males in the top dose group and 1 ad lib control rate died due to illness prior to breeding. Peak blood alcohol level was 338 +/- 15 mg% in the top

dose group and 132 +/- 5 mg% in the lower dose group. There were no adverse effects on male reproductive performance and female fecundity was no affected. Utter sizes and birth weights were not affected. Litter sizes and birth weights were not affected by paternal ethanol intake at either dose. Ethanol treatment in fathers had no effect on offspring growth rate.

There was a significantly higher number of female runts (bodyweight <5.5 g) in the groups sired by rats exposed to ethanol. There was also a significantly higher number of male runts in the groups sired by rats exposed to ethanol but only in comparison to the intubated control; the difference with the non-intubated control was not significant.

The % of males in litters sired by ethanol treated rats was significantly lower than the % sired by vehicle-treated fathers

	(p<0.04) although the difference with the non-intubated control was not significant. Ethanol treatment at both levels resulted in a significant increase in absolute adrenal gland weight but not in brain/bodyweight ratios. Organ weights (both absolute and bodyweight relative) were unaffected at 7 days but significant reductions of spleen and heart weight were noted at 21 days at the 3g/kg dose level (NOEL=2g/kg).
Conclusion	There was no effect on fertility in a group of 20 male rats given 3 g or 2 g/kg ethanol by oral intubation daily for nine weeks, achieving BAL's of 338±15 and 132±5 mg/dL, respectively. Although fertility was unaffected, this study did reveal higher incidences of runted pups in the resulting offspring especially at the highest exposure level (3g/kg).
Reliability	(2) valid with restrictions Study well enough reported for a valid with restrictions rating
Reference	Abel, E.L. (1993). Rat Offspring Sired by Males Treated with Alcohol. Alcohol 1993; 10: 237-242.
12.11.2004	(288)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Fertility
Species	Mouse
Sex	Male
Strain	C57BL
Route of admin.	oral feed
Exposure period	35 or 70 days
Frequency of treatm.	Daily
Doses	5 or 6% in feed calculated to yield 12,000 to 14,000 mg/kg/day
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Animals: supplied by Jackson Laboratories (Bar Harbor, ME). Age: 60 days. Environment 22 ± 1 degree C; relative humidity 45 ± 5%; 14 hr:10- hr lightdark cycle. Animals housed individually. Feed: Laboratory feed and water ad libitum. Treatment Vitamin supplemented (3g/l) chocolate flavoured Carnation Slender containing sucrose in amounts isocaloric to either 5% (v/v) or 6% (v/v) ethanol for 3 days after which on half of the animals in each group received diets containing 5% or 6% ethanol. All mice initially treated for 3 days on contra

	followed by 70 days treatment for the 5% ethanol group and 35 days for the 6% ethanol group. 48 Hr after cessation of treatment, mice were anaestheticsed then hemicastrated and the right testis and associated structures weight recorded. Spermatozoal function (number, motility, forward progression, in vitro fertilisation of mouse oocytes) and blood alcohol levels (BAL) were determined from 25ul aliquots of tail blood (head space sampling technique used). After castration, the incision was closed and the mice allowed free access to lab chow and water (no treatment) for a further 70 days. All animals then sacrificed. Group sizes consisted 5 to 12 individuals (treatment and control groups respectively). Controls: Vehicle (Carnation Slender containing sucrose as above). Statistical analysis: Wilcoxon tests; parametric data analysed following appropriate transformations and Newman-Keuls multiple range test.
Remark	Hemicastration was used to evaluate the reversibility of ethanol's effects on male reproductive function. Hemi-castrated pair fed controls were used to minimize the effect of hemicastration on the data (as it is known to produce compensatory effects on the remaining testis). Except for germ cell desquamation, all effects seen at the 5% ethanol diet were reversible. The authors speculated that Sertoli cells rather than Leydig cells are involved in reproductive failure of abstinent alcoholics.
Result	BAC peaked at 166± 38 mg% (1660 mg/l, n=15) for the 5% dose and 260± 35 mg% (2600 mg/l) for the 6% dose, both at day 34/35. After treatment with either 5%. ethanol or 6% ethanol, testicle weight decreased by 24% and 28%, but the effect was reversible and there was no significant difference between the control and recovery animals (10 weeks no treatment, P>0.1). Seminal vesicle/prostate weights decreased by 20% for those on the 6% diet but the effect was reversible and there was no significant difference between the control and recovery animals (10 weeks no treatment, P>O.1). There were significant increased frequencies of germ cell desquamation (480% in the 5% treatment group, 400% in the 6% treatment group) and of inactive seminiferous tubules (186% in the 5% treatment group, 567% in the 6% treatment group) Improvement in both parameters was noted in the contralateral organs after 10 weeks alcohol abstinence but all remained significantly elevated except for the % inactive tubules which returned to control group levels in the 5%

	treatment group. (Note: Germ cell desquamation in 5% treatment recovery group - 95% confidence limit range: 1.2-3.2% lumina showing desquamation versus control level of 0.31.0%.) Quality of spermatogenesis was significantly poorer in testes from both treatment groups compared to their respective controls. After 19 weeks abstinence, some pathology persisted in animals that had been exposed to ethanol although the differences were not significant. Caudal epididymal sperm content was not significantly affected by treatment with the 5% ethanol diet but was 6% lower in the animals receiving the 6% diet ($p<0.01$). This difference disappeared following 10 weeks without treatment. Sperm motility was not significantly affected by treatment with the 5% ethanol diet in the animals receiving the 6% diet molility was reduced by 85%. This difference disappeared following 10 weeks without treatment. Forward progression was reduced in both treatment groups (apparently more so in the lower treatment group). The difference disappeared in the recovery group that had been receiving 5% ethanol but persisted in the 6% group. In vitro fertilization of mouse oocytes by epididymal spermatozoa was reduced by 20% in the 5% treatment group and 63% in the 5% treatment group but these differences disappeared in both treatment groups following 10 weeks abstinence.
Source	IARC monographs on the evaluation of carcinogenic risk to humans. Vol 44, Alcohol Drinking. IARC, Lyon, France, 1988.
Conclusion	No NOAEL established (< 5% ethanol diet, <166 mg% BAC). However, for persistent effects the NOAEL would appear to be close to 5% ethanol diet.
Reliability	(2) valid with restrictions Not a standard study protocol but appears to be well conducted and reported. Limited and very high doses does not allow a NOAEL to be established.
Reference	Abel, E.L. (1993). Rat Offspring Sired by Males Treated with Alcohol. Alcohol 1993; 10: 237-242.
12.11.2004	(437)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Fertility
Species	Rat
Sex	Male
Strain	Sprague-Dawley
Route of admin.	Inhalation

Exposure period	3 to 4 weeks
Doses	22, 23, 25, 27 mg/l (approx 11500, 12000, 13000, 14000 ppm)
Control group	yes, concurrent no treatment
NOAEL parental	= 23 mg/l
NOAEL F1 offspring	= 25 mg/l
Method	other
Year	1983
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Animals: adults, 330-350 g; acclimated for 3-5 days. Animals housed together in airtight chambers. Controls: Housed in similar chambers to exposed animals without ethanol vapours present. Environment: Not described. Feed: Laboratory feed and water ad libitum during exposure. Feed supplemented with vegetables and peanut bars. Treatment: During acclimation, all treated rats were exposed to 22 mg/l ethanol vapour in air. After acclimation, groups of 10-12 rats were exposed to ethanol at 23, 25 or 37 mg/l for up to 3 to 4 weeks. Five exposure were run as separate experiments a concurrent controls. . After treatment, animals were immediately weighed then sacrificed and trunk blood collected over ice, the plasma separated and frozen for later analysis. Sex organs (testes, seminal vesicles, prostate) were removed and weighed. In one experiment, animals were injected with saline or gonadotropin releasing hormone (GnRH) and sacrificed 10 minutes later. Blood samples were withdrawn periodically from a tail vein for blood alcohol concentration (BAC) determination. Plasma testosterone and lutenising hormone (LH) were recorded. Statistical analysis: Dunnett's and Duncan's tests after analysis of variance.
Remark	This data supports the premise that fertility effects observed following high doses of ethanol may well be confounded by malnutrition stress.
Result	BACs of 94-127 mg/100ml resulted in smaller increase in bodyweight gain than observed in control animals but was not associated with significant changes in plasma testosterone levels or weights of sex organs. The maximum BAC observed was 187mg/100ml. A BAC of 180 mgl100 ml was associated with an inhibition of testosterone secretion only in animals that had failed to grow but this was not seen in a second experiment with a similar BAC.

In the experiment where GnRH was injected, a BAC of 163mg/100ml was associated with a marked weight loss and reduction of plasma testosterone levels. Basal plasma LH levels were comparable in the control and ethanol treated rats and intravenous administration of GnRH produced comparable

elevations in LH level in the controls and ethanol treated rats.

NOAEL (male fertility) = 127 mg/100 ml BAC LOAEL (male fertility) = 163mg/100 ml BAC Authors' conclusion is that data indicates that in growing animals testosterone secretion appears to be directly related to changes in body weight but not the degree of alcohol exposure. Adequate function of the hypothalamic-pituitary-testicular axis provided normal growth is maintained.
Alcohol does not appear to lower pituitary gland sensitivity to GnRH.

Reliability (2) valid with restrictions
Not a standard protocol but reasonably well reported and a no effect level established by a relevant route of exposure.

Reference Rivier C, and Vale W (1983). Influence of Ethanol on Reproductive Functions of the adult Male Rat as a Function of Body Weight. Alcohol: Clin Exp Res 1983; 7(3): 210-212.

12.11.2004 (289)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	One generation study
Species	Rat
Sex	Male
Strain	Sprague-Dawley
Route of admin.	Gavage
Exposure period	
Frequency of treatm.	Daily
Premating exposure period	
Male	3 and 9 weeks
Female	not treated
Duration of test	
No. of generation studies	1
Doses	2.5 and 5.0g/kg
Control group	yes, concurrent vehicle
Method	other
Year	1995
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)

Method	Animals: Supplied by Charles River, Portage, MI but test animals bred in laboratory. Age: 70 days. Number of animals: 18-26 per dose group. Environment: 22 ± t degree C; relative humidity 45 ± 5%; 12 hr:12 hr light:dark cycle. Feed: Laboratory feed and water ad libitum. Vehicle: distilled water. Controls: Vehicle (distilled water without ethanol) and non-intubated controls to evaluate the effects of intubation stress. Animals in the low and control treated groups were pair-fed to the high dose group animals. Treatment: Males were bred in once after 3 weeks exposure and twice after 9 weeks of exposure to 75-90-day-old females for 2 weeks or until sperm plugs were observed. Males were intubated throughout the mating period. Females with plugs were separated and housed individually. At 20 days gestation, females from the 3 week exposure breeding and one from the 9 week exposure breeding were killed and their foetuses counted, sexed and weighed. The second female from the 9 week breeding was allowed to deliver its litter, which was similarly assessed. Blood alcohol levels (BALs) were determined in males after 15 weeks exposure. Animals were sacrificed 1 hour after intubation (previously determined to coincide with peak BAL) and trunk blood measured. BAL was assessed by reduction of NAD by alcohol dehydrogenase using a Beckman automated analyser. Statistical analysis: Chi-square, ANOVA and Duncan Multiple Range Tests were used.
Remark	The 3 week exposure period was intended to assess the effect on postmeotic spermatids and spermatogonia whilst the 9 week exposure peroid was intended to assess the effect on germ cells throughout their maturation prior to as well as meiosis.
Result	Male fertility and litter size was not affected by treatment. Fecundity was not reduced in individual breedings but was significantly reduced at the 5g/kg dose level if the breeding periods were combined. There was no differences between the two control groups. At the first breeding (3 weeks) the 2.5g/kg and concurrent control males weighed significantly more than ad lib controls. After 9 weeks, only the concurrent control animals weighed significantly more than the ad lib controls. There did not appear to be any treatment related effects on resorptions and litter size. The mean BACs for the two ethanol dose groups was 248±14 mg% (5g/kg) and 155±9 mg%

	(2.5g/kg). There was:a treatment related increase in the number of male foetuses in the 3 week breeding at 5g/kg, but the effect was not repeated at the 9 week breedings. At the 3 and 9 week breedings there was a significant dose related increase in fetal weights. There was also a significant increase in placental weights, but only at the 9 week breedings. There were no treatment related effects on newborns sired by alcohol treated males.
Conclusion	There was no significant effect on male fertility. Female fecundity was reduced at the high dose level when all breedings were combined but litter size was not decreased nor were resorptions significantly increased. The main finding was an increase in fetal weights of offspring sired by alcohol treated males.
Reliability	(2) valid with restrictions Not a standard protocol but reasonably well reported. Dose levels very high and no clear "no effect level" established.
Reference	Abel (1995). A Surprising Effect of Paternal Alcohol Treatment on Rat Fetuses. Alcohol 1995; 12 (1): 1-6.
12.11.2004	(290)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Fertility
Species	Rat
Sex	male/female
Strain	Sprague-Dawley
Route of admin.	Inhalation
Exposure period	7 hours
Frequency of treatm.	Daily
Premating exposure period	
Male	6 weeks
Female	None
Duration of test	see method details
No. of generation studies	
Doses	0, 10000, 16000 ppm
Control group	Yes
NOAEL paternal	> 16000 ppm
Result	Negative
Method	other
Year	1985
GLP	no data

Test substance	95 – 99.9% ethanol (64-17-5)
Method	Exposure was conducted in 0.5m^3 chambers with dynamic air flow (one air change per minute.) Animals: 18/group. Starting weights 400-500g. Temperature: 73 +/- 3F. Humidity: average 40-50%. Exposure period: 2 day non exposure period before mating. Mating period 5 days. Mating confirmed by presence of sperm plugs under cages or vaginal smears. Females housed individually. Analytical monitoring: Yes (IR analyser - exposures found to be within 11 % of nominal). Independently cross-checked with charcoal adsorption tubes. Parameters measured: weights (daily), food and water intake.
Result	No effect on weight gain, feed or water intake. No effect on fertility or litter sizes. Previous studies quoted as showing exposures to 10000 and 16000 ppm ethanol typically give rise to blood ethanol concentrations of 30 and 500 mg/l ethanol. Authors calculate that for rats exposures in excess of 11000 ppm are required to begin accumulating ethanol in the blood and that ethanol is no more toxic by the inhalation route than by other routes.
Reliability	(2) valid with restrictions Well reported study but not to a standard protocol but no pathology on males. Study incomplete as a comprehensive assessment of effects on male fertility. Route of exposure highly relevant.
Reference	Nelson BK, Brightwell WS, Mackenzie-Taylor DR, Burg JR, Massari VJ (1988) Neurochemical but not behavioral deviations in the offspring of rats following prenatal or paternal inhalation exposure to ethanol. Neurotoxicol. Teratol. 10, 15-22. Nelson BK; Brightwell, WS, Burg JR (1985) Comparison of Behavioural Teratogenic Effects of Ethanol and n-propanol administered by inhalation to rats. Neurobehav. Toxicol. Teratol. 7, 779-83. Nelson, S., Brightwell, W., MacKenzie, D., et al. (1985). Teratological assessment of methanol and ethanol at high inhalation level in rats. Fundam. Appl. Toxicol. 5: 727-736.
12.11.2004	(291) (292) (293)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Fertility
Species	Rat
Sex	Female
Strain	CD-1
Route of admin.	S.C.
Exposure period	Once
Duration of test	Once
No. of generation studies	
Doses	7900 mg/kg bodyweight
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Ovulatory surges of LH and therefore ovulation were blocked by ethanol.
Reliability	(4) not assignable
Reference	Kieffer, J.D., Ketchel, M.M. Blockade of ovulation in the rat by ethanol. Acta. Endocrinol. 1970; 65: 117-124.
12.11.2004	(294)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Fertility
Species	Rat
Sex	Male
Strain	Sprague-Dawley
Route of admin.	Inhalation
Exposure period	1 week
Frequency of treatm.	6 hours/day
Doses	0, 1000 ppm
Year	1985
GLP	no data
Test substance	ethanol (64-17-5)
Method	Full method details provided in White (1983). Equilibrium concentrations achieved after 30 minutes. Temperature 20-22C, relative humidity 40-60% Controls: air only. No food or water during treatment. Statistical methods: student's t test, significant p<O.05 Animals sacrificed immediately after exposure or after an 18 hr rest period. Measurement of hormones was by radioimmunoassay.

Remark	Study designed to assess the effect on male reproductive function by quantifying serum concentrations of testosterone and luteinizing hormone.
Result	No significant effect on luteinising hormone or corticosterone. A significant depression of testosterone occurred after the first exposure, but the level returned to normal after 18hrs recovery and was absent at the end of the study.
Test substance	99% ethanol, supplied by Merck.
Conclusion	The relevance of this transient effect was not considered significant with respect to the ability of the testes to produce testosterone.
Reliability	(2) valid with restrictions Very restricted range of parameters assessed and exposure short. but within these restrictions, results appear reliable.
Reference	Cameron AM, Zahlsen K, Haug E, Nilsen OG, Eik-Ness KB (1985) Circulating steroids in male rats following inhalation of n-alcohols, Arch Toxicol Suppl 8, 422-4.
17.11.2004	(295)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	Fertility
Species	Monkey
Sex	Female
Strain	Macaca Fascicularis Lv.
Route of admin.	
Exposure period	3-6.5 months
Doses	2900-4400 mg/kg bodyweight
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Amennorrhea, atrophy of the uterus, decreased ovarian mass and significant lowering of LH levels were observed.
Reliability	(4) not assignable
Reference	Mello, N.K., Bree, M.P., Mendelson, J.H., Ellingboe, J. Alcohol self administration disrupts reproductive function in male Macaque monkeys. Science 1983; 221: 677-679.
12.11.2004	(296)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	One generation study

Species	Rat
Sex	male/female
Strain	Wistar
Route of admin.	oral feed
Exposure period	gestation day 12 to ten days postpartum
Duration of test	In utero and as neonates
No. of generation studies	
Doses	36% of calorie intake; estimated to be greater than 12,000 mg/kg/day
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	The authors concluded that there was less phenotypic masculinization at birth in the treated offspring.
Result	In male progeny there was decreased anogenital distance; the weights of the testes and seminal vesicles/prostate were decreased 55 and 110 days postpartum; serum testosterone and luteinizing hormone levels were decreased on day 55 but not on day 110; and sexual motivation and performance were reduced.
Reliability	(4) not assignable
Reference	Udani, M., Parker, S., Gavaler, J.S., Van Thiel, D.H. (1985) Effects of in utero exposure to alcohol upon male rats. Alcoholism Clinical and Experimental Research 9(4) 355-359.
12.11.2004	(297)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	One generation study
Species	Rat
Sex	Female
Strain	Wistar
Route of admin.	oral feed
Exposure period	while in utero and as neonates
Doses	36% of calorie intake
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Male offspring gonadal growth and sexual performance was adversely affected.

Reliability	(4) not assignable
Reference	Parker,S., Udani, M., Gavaker, J.S., Van Thiel, D.H.Adverse effects of ethanol upon the adult sexual behaviour of male rats exposed in utero. Neurobehav Toxicol Teratol 1984; 6: 289-293.
12.11.2004	(298)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	One generation study
Species	Rat
Sex	Female
Strain	Wistar
Route of admin.	drinking water
Exposure period	Before mating, through gestation and lactation
Doses	12% in drinking water
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	No effect on reproductive performance was noted.
Reliability	(4) not assignable
Reference	Oisund, J.F., Fjorden, A-E. and Moerland, J. Is moderate ethanol consumption teratogenic in the rat? Acta. Pharmacol. Toxicol. 1978; 43: 145-155.
12.11.2004	(299)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	One generation study
Species	Rat
Sex	Male
Strain	Sprague-Dawley
Route of admin.	i.p.
Exposure period	Once
Frequency of treatm.	Once
Doses	2500 mg/kg bodyweight
Control group	no data specified
Method	other
Year	

GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	There was a significant decrease in the level of LH and testosterone with marked attenuation of testicular steroidogenesis.
Reliability	(4) not assignable
Reference	Cicero, T,J., Meyer, E.R., Bell, R.D. Effects of ethanol on the hypothalamic- pituitaryluteinizing hormone axis and testicular steroidogenesis. J. Pharmacal. Exp. Ther. 1979; 208: 210-215.
12.11.2004	(300)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	One generation study
Species	Rat
Sex	Female
Strain	Wistar
Route of admin.	i.p.
Exposure period	
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Information taken from secondary source - no dosage information given.
Result	Ethanol increased prolactin secretion.
Reliability	(4) not assignable
Reference	Alfonso, M., Parafita, M.A., Mancebo, M.J., Marco, J. Further evidence for effects of ethanol on gonadotrophins and prolactin secretion in female rats. Gen Pharmacal 1985; 16 :43-47.
12.11.2004	(301)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Type	One generation study
Species	Rat
Sex	male/female
Strain	Sprague-Dawley
Route of admin.	Other
Doses	11600 mg/kg bodyweight
Control group	no data specified
Method	other

Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Patterns of LH secretion in both male and female offspring, as adults, indicated an effect on the central mechanisms controlling secretion of pituitary LH.
Reliability	(4) not assignable
Reference	Handa, R.J., et al. Exposure to alcohol in utero alters the adult patterns of luteinizing hormone secretion in male and female rats. Life Sci 1985; 37: 1683-1690.
12.11.2004	(302)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Type	One generation study
Species	Mouse
Sex	Female
Strain	C57BL
Route of admin.	drinking water
Exposure period	before mating, through gestation and lactation Daily
Frequency of treatm.	
Doses	10% in drinking water
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	No significant effect on reproductive capacity.
Reliability	(4) not assignable
Reference	Thiessen, D.O., Whitworth, N.S., Rodgers, D.A. Reproductive variables and alcohol consumption of the C57BI/Crgi female mouse. Q J Stud Alcohol 1966; 27: 591-595.
12.11.2004	(303)

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Species:	rat
Strain:	Sprague-Dawley
Sex:	male and female
Route of Admin.:	inhalation
Exposure Period:	Day 1-20 of gestation
Freq. of Treatment:	7 hours/day

Duration of Test:	20 Days
Exposure Concentrations:	0, 3000, or 6000 ppm of n-butanol. .
Control Group:	Yes
NOAEL Maternal Toxicity:	not reported
NOAEL Developmental Neurotoxicity:	6000 ppm
Method:	Groups of 18 male Sprague-Dawley rats were exposed to concentrations of 0, 3000, or 6000 ppm nBA for 7 hours/day for 6 weeks. These males were then mated to non-exposed female rats of the same strain. In a separate experiment, groups of 15 pregnant female rats were exposed to concentrations of 0, 3000, or 6000 ppm for 7 hours/day from gestation Day 1-20. These females were then allowed to deliver. The offspring from these two groups were then observed for signs of developmental neurotoxic effects. Offspring were examined from postnatal days 10-90 for the following measures: ascent on a wire mesh screen, rotorod, open-field and photoelectrically-monitored activity, running wheel, avoidance conditioning, operant conditioning, acetylcholine, dopamine, norepinephrine, serotonin, met-enkephalin, beta-endorphin, and Substance P. neurotransmitter levels were measured from the cerebrum, cerebellum, brainstem, and midbrain.
Year:	1989
GLP:	No
Test substance:	n-Butanol purity> 99%
Result:	No detectable effect on pregnancy rate was found after either maternal or paternal exposure. In the 6000 ppm group, 4 of the 78 (5%) behavioural measures, and 4 of the 64 (6%) neurochemical measures differed from those of controls. There was no discernible pattern of effects. The authors conclude, "In view of this, it is highly unlikely that administration of nBA at the current Permissible Exposure Limit (PEL) of 100 ppm would produce structural or behavioural teratogenicity in rats using the test employed here."
Reference:	Nelson, RK., Brightwell, W.S., Robertson, S.K., Kahn, A., Krieg, E.F., Ir. and Massari, V.I. Behavioral Teratology investigation of 1-Butanol in Rats. Neurotoxicology and Teratology. 11(3): 313-315, 1989a.

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Test substance:	1-Butanol, Analar reagent grade, from British Drug Houses, Ltd. (Poole, Dorset, England)
Species:	Rat (3-4 weeks old, 70-100 g)
Strain:	Sprague-Dawley
Sex:	Male 6/group

Route of Admin.:	Oral intubation, dissolved in corn oil
Exposure Period:	6 days
Freq. of Treatment:	Daily
Post Exposure:	None
Observation Period:	In-Life (6 days)
Doses:	533 mg/kg/day
Control Group:	Yes, vehicle control
NOAEL:	533 mg/kg/day
LOAEL:	>533 mg/kg/day
Test Method:	Research
Test Results:	Daily oral administration of dibutyl phthalate (DBP) at 2000 mg/kg/day for 4 days to young male rats was found to produce testicular injury, loss in testicular weight, and altered zinc metabolism. Monobutyl phthalate (MBP), the major metabolite of DBP, produced similar, but somewhat more potent, effects. Under similar treatment conditions, an equimolar dose of 1-Butanol (533 mg/kg/day) did not cause any effect on testes weight or histopathology.
GLP:	No
Comments:	Since 1-Butanol did not cause any effect on testes weight or histopathology, it was not tested for zinc metabolism.
Reference:	Cater et al., (1977). "Studies on Dibutyl Phthalate-Induced Testicular Atrophy in the Rat: Effect on Zinc Metabolism". Tax. and Applied Pharm., 41 :609-618.

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Test substance:	n-Butyl Acetate
Species:	Rat, male Sprague Dawley
Test Method:	Male ad libitum-fed rats were exposed via inhalation to 0, 500, 1500, or 3,000 ppm (6 hrs/day) for at least 65 exposures over 14 weeks. At necropsy, right testes (n=40) were prepared for histological examination and left testes and left epidymis (n=40) from the same animal were frozen and processed for determination of sperm concentrations.
Test Results:	Overall there was. no evidence of male reproductive toxicity at any exposure concentration based on lack of significant differences between treatments. and controls for testicular spermatid head counts and epididymidal spermatozoa counts as endpoints of toxicity. Therefore, a NOAEL for male reproductive toxicity following repeated exposure was 3000 ppm. Overall weight gains for 3000 ppm exposure groups were 64%

	and 59% of controls for males .and females, respectively. Overall weight gains for 1500 ppm exposure groups were 82% and 74% of controls for males and females, respectively. No significant differences in weight gain at 500 ppm vs. control.
GLP:	Yes
Comments:	Therefore, the NOAEL for male reproductive toxicity following repeated inhalation exposure with 3,000 ppm, the highest exposure tested. The rapid in vivo hydrolysis of n-butyl acetate to 1-butanol makes this study directly applicable to 1-butanol exposures.
Reference:	CMA Oxo-Process Panel; 1300 Wilson Blvd., Arlington Virginia 22209.

<u>1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)</u>

Test substance:	n-butanol
Species:	Rat, Imp:DAK; internal breeding colony to the Nufer Institute of Occupational Medicine in Lodz, Poland
Number of Animals:	11- 17/group
Route of Admin.:	Aqueous solutions for drinking water
Exposure Period:	8 weeks premating, 3 weeks mating, gestation Days 0-20
Frequency of Treatment:	Daily
Post Exposure:	None
Observation Period:	Premating (8 weeks), mating (up to 3 weeks), gestation (20 days)
Doses:	0.24, 0.8, or 4% n-butanol (0.3, 1.0, and 5.0 grams/kg/day)
Control Group:	Yes, vehicle control
NOAEL:	5.0 grams/kg/day
LOAEL:	>5.0 grams/kg/day
Test method:	Groups of 11-17 female rats were given aqueous solutions containing 0.24, 0.8, or 4% n-butanol for 8 weeks prior to mating, during which time estrous cyclicity was evaluated. After the 8 week exposure period (with no effects on estrous cyclicity), the females were mated with untreated males. The females had continued access to the solutions of n-butanol (above) in the water until Day 20 of gestation when they were killed and the fetuses were collected and examined for both skeletal and visceral malformations. Weight gains and feed consumption as well as general behavior were recorded during the 8 week premating period, 3 week mating period and gestation. The authors state that the aqueous solutions delivered 0.3, 1.0, and 5.0 grams/kg/day, although there is no information as to how this was determined. The 4% solution was. described as delivering daily doses twice as high as the acute oral LD50

(2.1 grams/kg/day). The unit of statistical analysis was the individual fetus, not the litter.

Test result: General appearance, feed consumption, body weights, rate of weight gain, estrous cycle length and number, absolute and relative organ weights (not specified), hemoglobin concentrations, hematocrit values, fetal body weights, intrauterine mortality, corpora lute a, total implants, and placental weights were unaffected.

GLP: No

Comments: While the developmental toxicity data from this papet is problematic due to poor reporting and study design, the reproductive data corroborate what was observed earlier by Nelson, et al., (1989a).

Reference: Sitarek, K., Berlinska, B., and Baranski, B. Assessment of the Effect of n-Butanol Given to Female Rats in Drinking Water on Fertility and Prenatal Development of Their Offspring. Int. J. of Occupational Medicine and Environmental Health, 7(4): 365-370, 1994.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Type: other: Repeat dose study with histopathology of reproductive organs.
Species: rat
Sex: male/female
Strain: other: Charles River
Route of administration: oral feed
Exposure Period: 13 weeks
Frequency of treatment: daily
Duration of test: 13 weeks
Doses: 0.25, 0.50, 1.0, 2.0, 4.0, and 6.0% w/w
Control Group: yes
NOAEL Parental: = 1127 - 1243 mg/kg bw

Method: other
Year: 1966
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Remark: These results were reported to USEPA in accordance with TSCA 8(e).

Result: None of the animals displayed gross effects of oral exposure to hexanol during the 13-weeks of the experiment. Food consumption and body weights were comparable to the controls.

No haematological changes were evident in any animals. Terminal organ weights (heart, spleen, gonads) were sporadically different from controls at different times. The original study report indicated significant differences between control and treated testes weights at all dose levels. No indication was given of which statistical method was used to analyse the data. Weinberg Associates reanalysed the data using a Tukey test and found that male gonad weights were not significantly different from the controls at any test concentration. There were no histopathological changes in any organs examined including the gonads. The NOAEL for reproductive endpoints is therefore the highest dose level (1243 mg/kg bw for females and 1127 mg/kg/day for males).

Source: Scientific Associates, Inc. 1966a.

Hayes Consultancy Service Bromley, Kent

Test condition: Groups of 20 rats (10 of each sex) were fed hexanol in the diet for 13 weeks. The control group consisted of 20 males and 20 females. The doses used were 0.25% w/w, low dose, 0.50% w/w, intermediate dose, and 1.00% w/w, high dose for weeks 1-10. They were fed 2.00% w/w for week 11, 4.00% w/w for week 12 and 6.00% w/w for week 13. At termination, all animals were sacrificed, necropsied, and tissues from 5 males and 5 females from the control and top dose groups were examined histopathologically. Fuller study details are reported in Chapter 5.4 Repeated dose toxicity.

Test substance: Tradename Alfol 6.

Conclusion: NOAEL for reproductive endpoints, 1243 mg/kg/day in females, 1127 mg/kg/day for males based on organ weights and histopathology of the gonads which showed no significant changes.

Reliability: (2) valid with restrictions
Study reasonably well documented, meets generally accepted scientific principles, acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: Scientific Associates, Inc. 1966a. Exhibit II. Final report on thirteen-week subacute feeding of Alfol 6 and Alfol 16 to rats.

07-SEP-2004 (60)

<u>1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)</u>

Type: other: Repeat dose study with histopathology of reproductive organs.

Species: dog

Sex: male/female

Strain: Beagle
Route of administration: oral feed
Exposure Period: 13 weeks
Frequency of treatment: daily
Duration of test: 13 weeks
Doses: 0.5, 1.0% w/w and 1000 mg/kg/day
Control Group: yes
NOAEL Parental: = 370 mg/kg bw

Method: other
Year: 1966
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Remark: These results were reported to USEPA in accordance with TSCA 8(e).
Result: In the highest level (~1100 mg/kg/day), all of the animals displayed signs of toxicity which consisted of salivation, excitation, ataxia, tremors, and anaesthesia and resulted in the death of both males and 2/3 females. There was also evidence of gastrointestinal inflammation and gonadal atrophy. Histopathological examination revealed testicular atrophy in the males which died and decreased oogenesis in one female. The ovaries of the surviving top dose female appeared normal. The gonadal changes were attributed to general ill health rather than direct toxic effects.
There were no adverse effects on the histopathology of the ovary or testes at the lower dose levels tested and no apparent effect on the organ weights. The value of this study is limited by the small numbers of animals used.
The NOAEL for reproductive endpoints was 370 mg/kg/day.
Source: Scientific Associates, Inc. 1966b.
Hayes Consultancy Service Bromley, Kent
Test condition: Groups of 4 Beagle dogs (2 of each sex) were exposed to 0.5, 1.0% w/w in the diet and 1000 mg/kg/day via gelatin capsule for 13 weeks. The control group contained 4 males and 4 females. At termination, all animals were sacrificed and necropsied. Full details of this study are reported in Chapter 5.4 Repeat dose toxicity.
Test substance: Tradename Alfol 6.
Conclusion: NOAEL 370 mg/kg/day (dietary administration of 1% test compound) for reproductive effects based on lack of histopathology in the gonads and no effect on reproductive organ weights. This was also the NOAEL for general systemic effects.
Reliability: (2) valid with restrictions

This study has methodological deficiences, animal group size

too small (only 2M+2F in test groups), no statistical analysis, high mortality in top dose level which was administered by capsule while lower dose levels were administered in the diet. Useful as supporting data.

Reference: Scientific Associates, Inc. 1966b. Exhibit III. Final report on thirteen-week subacute feeding in Beagle dogs of Alfol 6 and Alfol 16.

13-OCT-2004 (61)

1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)

Remark: The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C8 (1-octanol) alcohol is not expected to impair fertility are provided by lack of observed effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C) and similar negative data from the supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

Conclusion: Not expected to impair fertility.

Reliability: (2) valid with restrictions

The studies on which the conclusion for lack of potential for reproductive toxicity are based are either comparable to guideline studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

SIDS Dossier -Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

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Chain Alcohols (C6-22) including Iuclid dossiers chapter 5
prepared for the Aliphatic Alcohols category
14-SEP-2005 (104) (106) (119)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Remark: Reproduction: The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C10 alcohol (1-decanol) is not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D) and data from supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

Test substance: > 90% 1-decanol (112-30-1)
Conclusion: Not expected to impair fertility.
Reliability: (2) valid with restrictions
The studies on which the conclusion for lack of effect on the reproductive potential is based are either comparable to guideline studies or publications with sufficient detail for assessment.
Reference: SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category
12-SEP-2005 (84) (85) (97)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Type	:	other: Combined repeat dose and Reproductive/Developmental screening study
Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	oral feed
Exposure period	:	Males 41-44 days , females up to 54 days
Frequency of treatment	:	continuous in diet
Premating exposure period		
Male	:	14 days
Female	:	14 days
Duration of test	:	Males 41-44 days , females up to 54 days
Doses	:	0, 100, 500, 2000 mg/kg bw/day
Control group	:	yes
NOAEL Parental	:	= 2000 mg/kg bw
NOAEL F1 Offspr.	:	= 2000 mg/kg bw
Method	:	other: Combined repeat dose and reproductive/developmental toxicity screening test
Year	:	1992
GLP	:	yes
Test substance	:	dodecanol (112-53-8)
Test condition	:	TEST ORGANISMS: Rat Wistar aged 8 (males) - 9 (females) weeks at start of exposure period. 12M+12F/group ADMINISTRATION / EXPOSURE - Type of exposure: Dietary - Duration of test/exposure: males 41-44 days, females approx. 54 days - Treatment: - Control group and treatment: - Vehicle: Diet - Concentration in vehicle: 0, 1500, 7500 & 30,000 ppm MATING PROCEDURES: 14 day premating exposure, then 1M+1F caged together. Inspection for vaginal plugs thrice daily. If mating did not occur after 14 days cohabitation the female was placed with another male for 8 days. STANDARDIZATION OF LITTERS: No PARAMETERS ASSESSED DURING STUDY P:

- Clinical observations: body weight, weight gain, food consumption, food efficiency.
- Estrous cycle: Exposure was for 14 days premating covering at least 2 oestrous cycles. Ovaries were weighed and examined histopathologically at section (21 days after birth).
- Sperm examination: Exposure 14 days premating, no specific sperm analyses carried out, the testes & epididymes were weighed and examined histopathologically.
- Reproductive parameters: Pregancy rate, length of gestation, implantations, corpora lutea and resorptions were recorded.

OFFSPRING: Offspring (and dams) were sacrificed on post natal day 5 and the pups were weighed and examined for external malformations than sexed and examined for internal malformations.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights P: liver, kidneys, thymus, testis, epididymes.
- Histopathology P: liver, kidneys, adrenals, brain, heart, spleen, ovaries, thymus, testes, epididymides and any organs showing abnormality on macroscopic examination were fixed. The above tissues from all controls and top dose treated rats (except the thymus) plus abnormalities were examined.
- Macroscopic P: Full macroscopic examination.

OTHER EXAMINATIONS: Haematological and biochemical parameters were measured for the Repeat dose toxicity assessment, full details in Chapter 5.4 Repeat dose toxcity

STATISTICAL METHODS: Analysis of variance followed if significant differences were established by Dunnetts T-test to assess possible intergroup differences. For pregnancy rate a Qui2-test was carried out to confirm lack of significance.

Result : NOAEL: 2000 mg/kg/day (highest dose tested) for systemic and reproductive toxicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 100, 500 and 2000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Parental data and F1:
- Body weight: No treatment related effects.
- Food/water consumption: No treatment related effects.
- Description, severity, time of onset and duration of clinical signs: None reported.

- Pregancy rate: There was no statistically significant difference in pregancy rates although they were reduced in treated groups C 92%, 100 & 500 mg/kg 83%, 2000 mg/kg/day 75% these were within the normal historical control range according to the authors (actual historical control data not presented).
- Fertility index: Not reported
- Precoital interval: Not reported
- Duration of gestation: Comparable in treated and control dams (23 days in all groups).
- Gestation index: Not reported
- Changes in lactation: Not reported
- Changes in estrus cycles: Not reported
- Effects on sperm: Not reported
- Clinical biochemistry findings incidence and severity: (males only investigated) None considered of biological significance see Chapter 5.4 Repeated dose toxicity for fuller details.
- Haematological findings incidence and severity: (males only investigated) None considered of biological significance see Chapter 5.4 Repeated dose toxicity for fuller details.
- Organ weights: There were no statistically significant dose related changes in organ weights including the testes, epididymes and ovaries.
- Gross pathology: There were no changes attributable to exposure to the test compound.
- Histopathology: There were no treatment related histopathological changes including no effects in the testes and ovaries.
- Mortality: None
- Number of implantations: No significant differences in the numbers of implantations between treated and control groups (mean 13 in control group, 14 in each treated group). There were no resorptions.
- Number of corpora lutea: No significant differences between treated and control groups (mean 14 in test and controls).
- Ovarian primordial follicle counts: Not reported
- Offspring toxicity F1:
- Litter size and weights: No effect of treatment. Litter size mean Controls 13.25, low dose 13.27, mid dose 13.2, high dose 13.33. Mean litter weights at day 1 were 75, 75, 71 and 77 gm and at day 4 106, 107, 101 and 104 gm for control, low, mid and high dose respectively. No statistical significance.
- Sex and sex ratios: No treatment related effects.
- Post natal survival until day 5: Similar in treated and control groups.

Conclusion : Parental NOAEL 2000 mg/kg/day. No adverse effects were observed on reproductive parameters and the NOAEL for reproductive and developmental effects can also be considered to be 2000 mg/kg/day.

Reliability	:	(2) valid with restrictions Comparable to guideline study (draft guideline) with acceptable restrictions
Source	:	Hansen 1992a. Hayes Consultancy Service Bromley, Kent
Flag	:	Critical study for SIDS endpoint
Reference		Hansen, E. 1992a. Combined repeat dose and reproductive/developmental toxicity screening test on 1-dodecanol in rats. Institut of Toxicology, Danish National Food Agency, IT 921105.
11.08.2005		(9)

<u>1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)</u>

Remark: The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C14 alcohol (tetradecanol) is not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving C10-16 alcohols (types B&D), C14-16 (type A), C16 (hexadecanol) and from the supporting substance C18 (octadecanol).

Source: Hayes Consultancy Service Bromley, Kent

Test substance: > 95% 1-Tetradecanol (112-72-1)

Conclusion: Not expected to impair fertility.

Reliability: (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic

alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category
15-SEP-2005 (66) (67) (78)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Type: other: Repeat dose study with histopathology of reproductive organs.
Species: rat
Sex: male/female
Strain: other: Charles river
Route of administration: oral feed
Exposure Period: 13 weeks
Frequency of treatment: continuous
Duration of test: 13 weeks
Doses: 1.0% and 2.5% for 13 weeks, 5.0% for 10 weeks then 7.5% week 11 and 10.0% weeks 12 & 13.
Control Group: yes
NOAEL Parental: = 1822 mg/kg bw

Method: other
Year: 1966
GLP: no
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: These results were reported to USEPA in accordance with TSCA 8(e).
Result: None of the animals displayed overt signs of intoxication due to oral exposure to hexadecanol during the 13 weeks of the experiment. Food consumption and body weights differed significantly for both males and females at various times in the intermediate and high dose levels. The relative testes weights were increased over control levels in all treatment groups reaching signficance in the low and high group according to the study report. The organ weight data were reanalysed by the Weinberg Associates using a Tukey test when significance was attained only at the high dose level. There were no significant changes in ovary weight. Histopathological examination revealed no treatment related changes in the ovaries or testes. The NOAEL for effects on the male reproductive organs can be considered as a dietary concentration of 2.5% (ca 2000 mg/kg/day) the NOAEL for the female reproductive organs is the highest dose level (ca 4000

mg/kg/day). Actual dose levels achieved at respective NOAELs, males 1822 mg/kg/day and females 4567 mg/kg/day. Full study report is to be found in Chapter 5.4 Repeated dose toxicity.

Source: Scientific Associates, Inc. 1966a.

Hayes Consultancy Service Bromley, Kent

Test condition: Groups of 20 rats (10 of each sex) were fed Alfol 16 in the diet for 13 weeks. The control group consisted of 20 males and 20 females at dose levels of 1, 2.5 and 5% with the top dose level increasing at week 11 to 7.5% and for weeks 12& 13 to 10% in the diet. At termination, all animals were necropsied and tissues from 5 males and 5 females (including gonads) of the high dose group and a similar number of controls were examined histopathologically. Testes and ovary weights were recorded together with other organ weights. For full experimental details see Chapter 5.4 Repeat dose toxicity.

Test substance: Tradename Alfol 16

Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

Reference: Scientific Associates, Inc. 1966a. Exhibit II. Final report on thirteen-week subacute feeding of Alfol 6 and Alfol 16 to rats.

06-AUG-2005 (77)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Type: other: Repeat dose study with histopathology of reproductive organs.
Species: dog
Sex: male/female
Strain: Beagle
Route of administration: oral feed
Exposure Period: 13 weeks
Frequency of treatment: daily
Duration of test: 13 weeks
Doses: 0.5, 1.0 and 3.0% w/w
Control Group: yes
NOAEL Parental: > 1054 mg/kg bw

Method: other
Year: 1966
GLP: no data
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Remark: These results were reported to USEPA in accordance with TSCA 8(e).

Result: There were no overt signs of toxcity and no treatment related histopathological changes. There were no adverse effects on male or female reproductive organs as evidenced by lack of effect on gonad weights and lack of histopathological changes in the gonads of the high dose animals. The value of this study is limited by the small numbers of animals used.

Source: Scientific Associates, Inc. 1966b.

Hayes Consultancy Service Bromley, Kent

Test condition: Groups of beagle dogs (2 of each sex/dose level) were exposed to hexanol at dose levels of 0.5, 1.0% and 3% w/w in the diet for 13 weeks. The control group contained 4 males and 5 females. Full details of this study are reported in Chapter 5.4 Repeat dose toxicity. Testes and ovaries were weighed and organs from top dose dogs examined histopathologically.

Test substance: Tradename Alfol 16

Conclusion: The NOAEL for effects on the reproductive organs of dogs is >1054 mg/kg/day (3% in the diet). There were no treatment related effects on reproductive organ weights and no histopathological changes in the gonads of top dose animals. This is also the NOAEL for systemic toxicity.

Reliability: (2) valid with restrictions

Reliability 2 however there were methodological deficiencies, animal group size too small (2M + 2F in test groups), no statistical analysis in original study, subsequent analysis by The Weinberg Group Inc of limited relevance because of small group sizes.

Reference: Scientific Associates, Inc. 1966b. Exhibit III. Final report on thirteen-week subacute feeding in Beagle dogs of Alfol 6 and Alfol 16.

06-AUG-2005 (78)

<u>1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)</u>

Type: other: Repeat dose study with histopathology of reproductive organs.

Species: rat

Sex: male/female

Strain: Sprague-Dawley

Route of administration: gavage

Exposure Period: 28 days

Frequency of treatment: daily

Duration of test: 28 days

Doses: 100, 500, and 1000 mg/kg bw

Control Group: yes

NOAEL Parental: = 1000 mg/kg bw

Method: other: An in-house protocol based on OECD Guide-line 407
Year: 1985
GLP: no data
Test substance: >= 95% 1-hexadecanol (36653-82-4)

Result: There were no deaths among the test animals. Food intake, water consumption, body weight, organ weight, and haematological parameters were not affected.
The absolute and relative organ weights of the ovary and testes were determined and were comparable to controls.
Reproductive tissues from the control and top dose animals (1000 mg/kg/day were examined histopathologically. In females examination of the ovaries, uterus and vagina and in males histopathological examination of the testes and prostate showed no difference between treated and control groups. The NOAEL for effects on the reproductive organs was considered to be 1000 mg/kg/day.
Source: Henkel KGaA 1999 (English summary); Henkel 1985a is the original report in German
Hayes Consultancy Service Bromley, Kent
Test condition: Groups of 10M+10F rats received daily doses of 0, 100, 500 and 1000 mg/kd Lanette 16 by gavage for 28 days. Full details of this study are reported in Chapter 5.4 Repeated dose toxicity.
The testes and ovaries were weighed and these organs plus the prostate, uterus and vagina from all control and top dose animals were subject to histopathological examination.
Test substance: Tradename Lanette 16
Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
Reference: Henkel KGaA. 1985a. Lanette 16: 28-Tage-Test mit wiederholter oraler Verabreichung an Ratten. November 1985. Report No. TBD 850499. With pathology report No. 840394.
06-AUG-2005 (41)

<u>1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)</u>

Type	:	other: Combined repeat dose and Reproductive/Developmental screening study.
Species	:	rat
Sex	:	no data
Strain	:	Wistar
Route of admin.	:	oral feed
Exposure period	:	males 45 days,up to 54 days
Frequency of treatment	:	continuous in diet

Premating exposure period		
Male	:	14 days
Female	:	14 days
Duration of test	:	males 45 days,up to 54 days
Doses	:	0, 100, 500, 2000 mg/kg/bw/day
Control group	:	yes
NOAEL Parental	:	= 2000 mg/kg bw
NOAEL F1 Offspr.	:	= 2000 mg/kg bw
Method	:	other: Combined repeated dose and reproductive/developmental toxicity screening test
Year	:	1992
GLP	:	yes
Test substance	:	other TS: Octadecanol (112-92-5) (99% pure)
Test condition	:	TEST ORGANISMS: Rat Wistar aged 8 (males) - 9 (females) weeks at start of exposure period. 12M+12F/group ADMINISTRATION / EXPOSURE - Type of exposure: Dietary - Duration of test/exposure: males 45 days, females up to 54 days - Vehicle: Diet - Concentration in vehicle: 0, 1500, 7500 & 30,000 ppm MATING PROCEDURES: 14 day premating exposure, then 1M+1F caged together. Inspection for vaginal plugs thrice daily. If mating did not occur after 14 days cohabitation the female was placed with another male for 8 days. STANDARDIZATION OF LITTERS: No PARAMETERS ASSESSED DURING STUDY P: - Clinical observations: body weight, weight gain, food consumption, food efficiency. - Estrous cycle: Exposure was for 14 days premating covering at least 2 oestrous cycles. Ovaries were weighed and examined histopathologically at section (5 days after birth). - Sperm examination: Exposure 14 days premating, no specific sperm analyses carried out, the testes & epididymes were weighed and examined histopathologically. - Reproductive parameters: Pregancy rate, length of gestation, implantations, corpora lutea and resorptions were recorded. OFFSPRING: Offspring (and dams) were sacrificed on post natal day 5 and the pups were weighed and examined for external malformations than sexed and examined for internal malformations.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights P: liver, kidneys, thymus, testis, epididymes.
- Histopathology P: liver, kidneys, adrenals, brain, heart, spleen, ovaries, thymus, testes, epididymides and any organs showing abnormality on macroscopic examination were fixed. The above tissues from all controls and top dose treated rats (except the thymus) plus abnormalities were examined.
- Macroscopic P: Full macroscopic examination.

OTHER EXAMINATIONS: Haematological and biochemical parameters were measured for the Repeat dose toxicity assessment, full details in Chapter 5.4 Repeat dose toxcity

STATISTICAL METHODS: Analysis of variance followed if significant differences were established by Dunnetts T-test to assess possible intergroup differences. For pregnancy rate a Qui2-test was carried out to confirm lack of significance.

Result : NOAEL: 2000 mg/kg/day (highest dose tested) for systemic and reproductive toxicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 100, 500 and 2000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Parental data and F1:
- Body weight: No treatment related effects.
- Food/water consumption: No treatment related effects.
- Description, severity, time of onset and duration of clinical signs: None reported.
- Pregancy rate: There was no statistically significant difference in pregnancy rates (confirmed using a Qui2-test) although they were reduced in treated groups C 92%, 100 & 500 mg/kg 75%, 2000 mg/kg/day 67% these were within the normal historical control range according to the authors (actual historical control data not presented).
- Fertility index: Not reported
- Precoital interval: Not reported
- Duration of gestation: Comparable in treated and control dams (mean 22 days for all groups).
- Gestation index: Not reported
- Changes in lactation: Not reported
- Changes in estrus cycles: Not reported
- Effects on sperm: Not reported

- Clinical biochemistry findings incidence and severity: (males only investigated) None considered of biological significance see Chapter 5.4 Repeated dose toxicity for fuller details.
- Haematological findings incidence and severity: (males only investigated) The significance of changes in plasma free cholesterol, triglycerides and glucose is unclear, the changes were observed at all doses levels but were not dose related. They may be related to differences in dietary composition. See Chapter 5.4 Repeated dose toxicity for fuller details.
- Organ weights: There were no statistically significant dose related changes in organ weights including the testes, epididymes and ovaries.
- Gross pathology: There were no changes attributable to exposure to the test compound.
- Histopathology: There were no treatment related histopathological changes including no effects in the testes and ovaries.
- Mortality: None
- Number of implantations: No significant differences in the numbers of implantations between treated and control groups)Mean 13 in controls and low dose, 15 in mid and high dose groups). Resorptions mean for controls and low dose 0, for mid and high dose 1).
- Number of corpora lutea: No significant differences between treated and control groups (mean controls 13, low and mid dose 14, high dose 15).
- Ovarian primordial follicle counts: Not reported
- Offspring toxicity F1:
- Litter size and weights: No effect of treatment (mean liter size 11.73, 10.0, 13.6 and 13.38 for controls, low, mid and high dose respectively).
Letter weights day 1 mean 69, 61, 75 and 75 gm; Day 4 mean 96, 84, 101 and 101gm for controls, low, mid and high dose respectively)
- Sex and sex ratios: No treatment related effects.
- Post natal survival until day 5: Similar in treated and control groups.

Conclusion : Parental NOAEL 2000 mg/kg/day changes in plasma free cholesterol, triglycerides and glucose were observed at all doses levels but were not dose related and may be due to differences in dietary composition. There were no statistically significant adverse effects on reproductive parameters and the NOAEL for reproductive and developmental effects can be considered as 2000 mg/kg/day (highest dose level).

Reliability : (2) valid with restrictions
Comparable to guideline study (draft guideline) with acceptable restrictions

Source : Hansen 1992b.

		Hayes Consultancy Service Bromley, Kent
Flag	:	Critical study for SIDS endpoint
Reference		Hansen, E. 1992b. Combined repeat dose and reproductive/developmental toxicity screening test on 1-octadecanol in rats. Denmark: Institute of Toxicology, National Food Agency, IT 911130.
08.01.2006		(9)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Type	:	other: Repeat dose study with histopathology of reproductive organs.
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	28 days
Frequency of treatment	:	daily 5 days/week
Premating exposure period		
Male	:	
Female	:	
Duration of test	:	
Doses	:	0, 100, 500, and 1000 mg/kg in olive oil
Control group	:	yes
NOAEL Parental	:	= 1000 mg/kg bw
Method	:	other: OECD Guideline 407
Year	:	1996
GLP	:	yes
Test substance	:	octadecanol (112-92-5)
Test substance	:	Tradename Lanette 18
Test condition	:	Groups of 10M+10F rats received daily doses of 0, 100, 500 and 1000 mg/kd Lanette 18 by gavage for 28 days. Full details of this study are reported in Chapter 5.4 Repeated dose toxicity. The testes and ovaries were weighed and these organs plus the prostate and uterus from all control and top dose animals were subject to histopathological examination.
Result	:	No animals died during the test. Food intake and water consumption were comparable to the control group. Body weight gain and total increase of body weights did not differ from control values. There were no significant differences in the weight of the testes or ovaries. Histopathological examination of the testes, prostate, ovaries and uterus revealed no treatment related changes. NOAEL for effects on

the reproductive organs 1000 mg/kg/day.

Reliability : (1) valid without restriction
Guideline study

Source : Henkel KGaA 1986a
Hayes Consultancy Service Bromley, Kent

Reference Henkel KGaA. 1986a. Lannette 18: 28-Tage-Test mit wiederholter oraler Verabreichung an Ratten. Report No. TBD 860071. Institut fur Toxikologie. With pathology report No. 840230

Henkel KGaA. 1999. Octadecanol: Evaluation of repeated dose oral toxicity. Unpublished data, English summary and evaluation of Report No. TBD 860071.

12.08.2005 (13) (14)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Remark: The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C20 alcohol (eicosanol) is not expected to impair fertility are provided, in addition to the negative reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving C16 (hexadecanol), C22 (docosanol) and the supporting substances C18 (octadecanol) and C24-34 alcohols.

Test substance: >= 90% 1-eicosanol (629-96-9)

Conclusion: Not expected to impair fertility.

Reliability: (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long

Chain Alcohols (C6-22) including Iuclid dossiers chapter 5
prepared for the Aliphatic Alcohols category
15-SEP-2005 (18) (23)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Type: other: fertility and reproductive toxicity
Species: rat
Sex: male/female
Strain: Sprague-Dawley
Route of administration: gavage
Exposure Period: Males for 71 days prior to mating until females were sacrificed. Females for 15 days prior to mating, during mating, and up to Day 17 of gestation.
Frequency of treatment: daily
Premating Exposure Period
male: 71 days
female: 15 days
Duration of test: 20th day of gestation
No. of generation studies: 1
Doses: 10, 100, 1000 mg/kg bw-day
Control Group: yes
NOAEL Parental: = 1000 mg/kg bw
NOAEL F1 Offspring: = 1000 mg/kg bw

Method: other: see text
Year: 2000
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)

Result: NOAEL: P1 and F1 1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 10, 100 and 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Parental data and F1: None
- Body weight: Comparable between test and control groups.
- Food/water consumption: Comparable between test and control groups.
- Description, severity, time of onset and duration of clinical signs: One top dose male was sacrificed during week 6. There were no other remarkable clinical observations and the single death was not attributed to treatment.
- Fertility index: Not calculated
- Pregnancy rate: Number of pregnant animals 22, 22, 22 and 21 for controls, low, mid and high dose respectively.

- Precoital interval: Not reported.
- Duration of gestation: Comparable between treated and control groups.
- Gestation index: not calculated.
- Effects on sperm: No adverse effects.
- Hematological findings incidence and severity:
- Clinical biochemistry findings incidence and severity:
- Mortality: One top dose male was sacrificed during week 6.
- Gross pathology incidence and severity: Comparable in treated and control groups.
- Number of implantations: No significant difference between treated and controls. Implantations (mean) 17.2, 17.0, 18.1 and 18.0 for controls, low, mid and high dose respectively; Preimplantation loss 3.3, 8.3, 3.2, 5.8%; Postimplantation loss 4.7, 6.4, 6.3 and 5.8% for controls, low, mid and high dose respectively.
- Number of corpora lutea: No significant difference between treated and controls. Mean corpora lutea 17.8, 18.4, 18.7 and 18.9 for controls, low, mid and high dose respectively.
- Organ weight changes: No significant difference between treated and controls.
- Offspring toxicity F1 (gestation day 20):
- Litter size and weights: Comparable between treated and controls
- Sex and sex ratios: Comparable between treated and controls
- Viable young: Comparable between treated and controls. Viable young (mean) 16.4, 15.9, 17.0 and 16.9 for controls, low, mid and high dose respectively.
- Foetal examination: No macroscopic, internal or skeletal malformations or variations outside of historical control limits.

Source: Iglesias, 2002b
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS
Age/weight at study initiation: males 6-7 weeks old, 193-240g; females 10-11 weeks old, 208-262g
Number of animals: Groups of 22M+22F per dose level.

ADMINISTRATION / EXPOSURE
- Type of exposure: Gavage
- Duration of test/exposure: males 71 days premating until sacrifice of females (day gestation day 20), females 15 days premating until day 17 of gestation.
- Treatment: 0,10, 100 or 1000 mg/kg/day
- Control group and treatment: vehicle control
- Vehicle: 1% aqueous Tween 80
- Concentration in vehicle: 20% stock diluted to give standard

dosing volume.
- Total volume applied: 5 ml/kg
- Doses: 0, 10, 100 and 1000 mg/kg/day

MATING PROCEDURES: males & females caged 1:1 during mating period, length of mating period unspecified.

STANDARDIZATION OF LITTERS: No

PARAMETERS ASSESSED DURING STUDY P:
- Clinical observations: Daily clinical signs, food & water consumption premating weekly (males), daily (females); gestation females (food & water) GD 0-2, 3, 6, 7-9, 10-13, 14-17 and 18-19. Body weights premating twice weekly F, then at GD 0, 3, 7, 10, 14, 18 and 20. Males twice weekly throughout exposure period. Complete macroscopic examination.
- Estrous cycle: Assessed by daily vaginal smears for 10 days prior to mating.
- Sperm examination: At the end of the study, a sperm count and measurement of sperm motility was carried out.
- Reproductive parameters: corpora lutea, pre & post impalntatons sites, early & late resorption sites, viable foetuses, position of foetuses in uterine horns

OFFSPRING: Examined at day 20 of gestation. Placental weights, viable foetuses, skeletal & visceral examination.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights P: males reproductive organs

STATISTICAL METHODS: one way analysis of variance and T-test on body weights, food & water consumption. Organ weights - Dunnetts or Behren's-Fischer's test. Nested analysis of variance and weighed t-test for fetal and palcental weights.

Test substance: C22 alcohol CAS RN 661-19-8 (behenyl alcohol)

Conclusion: NOAEL for reproductive effects 1000 mg/kg/day. There were no treatment related adverse effects on reproductive parameters at any dose level.

Reliability: (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).

Flag: Critical study for SIDS endpoint

Reference: Iglesias, G, JJ Hlywka, JE Berg, MH Khalil, LE Pope and D Tamarkin. 2002b. The toxicity of behenyl alcohol: II. Reproduction studies in rats and rabbits. Regulatory Tox. and Pharm. 36, 80-85.

1-Tetracosanol, 1-Hexacosanol, 1-Octacosanol, and 1-Triacontanol for their respective Aluminum Salts

Type	:	other: Repeat dose study with histopathology of reproductive organs.
Species	:	dog
Sex	:	male/female
Strain	:	Beagle
Route of admin.	:	gavage
Exposure period	:	1 year
Frequency of treatment	:	daily
Premating exposure period		
Male	:	
Female	:	
Duration of test	:	1 year
Doses	:	50, 250 mg/kg bw
Control group	:	yes
NOAEL Parental	:	= 250 mg/kg bw
Method	:	other
Year	:	2001
GLP	:	no data
Test substance	:	C24-C34 alcohol
Test substance	:	A C24-C34 alcohol, called D-002, primarily isolated and purified from beeswax. The composition is C24 (13.2%), C26 (15.3%), C28 (17.5%), C30 (26.6%), C32 (17%), C34 (2.2%) and 7% of "other well known, non-active substances". C24-34 even alcohol (D-002)
Test condition	:	Groups of 4M + 4F dogs received 0, 50 or 250 mg/kg/day by gavage for a year. Full details of this study are to be found in Chapter 5.4: Repeated dose toxicity. Weights of the testes and prostate gland were measured and the testes, prostate, penis, ovaries, uterus and vagina were examined histopathologically.
Result	:	No deaths occurred during the study. There were no clinical symptoms of toxicity observed and no significant difference in body weight gain between controls and test animals. Testes weight in treated groups was comparable to that of the controls. Ovaries were not weighed. Histopathological examination of the reproductive organs in both sexes revealed no treatment related changes. The NOAEL for effects on the reproductive organs is 250 mg/kg/day
Reliability	:	(2) valid with restrictions

		Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment.
Source	:	Aleman 2001. Hayes Consultancy Service Bromley, Kent
Reference		Aleman, C., Rodeiro, I., Noa, M., Menendez, R., Gamez, R., Hernandez, C., and Mas, R. 2001. One-year dog toxicity study of D-002, a mixture of aliphatic alcohols. J. Appl. Toxicol. 21: 179-184.
24.01.2005		(1)

5.8.2 Developmental Toxicity/Teratogenicity

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	Female
Strain	Sprague-Dawley
Route of admin.	Inhalation
Exposure period	17 hours per day
Frequency of treatm.	Daily
Duration of test	Days 1-19 of gestation
Doses	10,000,16,000 or 20,000 ppm
Control group	no data specified
NOAEL maternal tox.	= 16000 ppm
NOAEL teratogen.	> 20000 ppm
LOAEL Maternal Toxicity	= 20000 ppm
LOAEL Teratogenicity	>= 20000 ppm
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	Age at study start - not stated - 176-200 g. Number of animals per dose per sex: not explicitly stated but approximately 16. Doses are calculated to be equivalent to 17, 29 and 28 g/kg bodyweight. Vehicle used - not applicable Mating conditions: Virgin females were housed with males and vaginal smears were taken. Foetuses were examined externally and internally for malformations; implants and resorptions were recorded as was litter weight.

No maternal organs were examined and fetuses were examined for external and visceral malformations.
Maternal LOAEL effect was narcosis and lowered food consumption.
Development LOAEL effect - none seen Development NOAEL effect - visceral or skeletal malformations or variants.
Statistical tests were t-tests or chi-square tests; p=<O.05 regarded significant.
This was considered in the IARC Monograph 1988.

Result

No mortality occurred.

Maternal data are not given for the following:

Number aborting Number of corporea lutea (Duration of pregnancy not relevant) Bodyweights Haematology and blood chemistry findings Gross pathology in dams Organ weight changes Histopathology incidence and severity.

Maternal data are given for the following:

The number of pregnant per dose level were 15/15, 15/16 and 14/16 in the low, medium and high dosage groups.
The numbers of resorptions were not affected by ethanol inhalation.
Number of implantations were 14-16/litter in all ethanol-treated groups.
Number of corpora lutea were 14-16/1itter Food consumption was lowered in the high-dose group.
Clinical signs: the highest dose induced complete narcosis (described as severe toxicity); lower doses did not cause narcosis but caused hyperactivity after exposure.
Maternal weight gains were not affected by treatment.

Blood alcohol levels ranged 0.02 to 0.04 mg/ml at 10000ppm, 0.43 to 0.53 mg/ml at 16000ppm and 1.48 to 1.93 mg/ml at 20000ppm. Measurements were made on non-pregnant rats and represent the ranges of the average values measured at days 1, 10 and 19.

Foetal data are not given for the following:

Litter size (but are deduced to average 6.0 to 7.1 foetuses/litter across the groups).
Number viable Postnatal growth (not applicable) Postnatal survival (not applicable)

	Foetal data are given for the following: Utter weights were not significantly affected by ethanol treatments. Sex ratio did not differ significantly from controls. Grossly visible abnormalities are given in detail but the frequency of each did not differ significantly between groups. More litters contained abnormal foetuses in the 20,000 ppm group compared to controls.
Conclusion	No definite evidence of malformations due to ethanol exposure were seen although the incidence of abnormal changes at the highest concentration was of borderline significance.
Reliability	(2) valid with restrictions Well reported study which established a NOAEL
Flag	Critical study for SIDS endpoint
Reference	Nelson, B., Brightwell, W., MacKenzie, D., et al. (1985). Teratological assessment of methanol and ethanol at high inhalation level in rats. Fundam Appl Toxicol. 5: 727-736.
12.11.2004	(293)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	male/female
Strain	Wistar
Route of admin.	Gavage
Exposure period	throughout gestation and gestation + lactation
Frequency of treatm.	Daily
Duration of test	
Doses	1 g/kg/day (12.5% v/v in distilled water)
Control group	yes, concurrent vehicle
Method	other
Year	1998
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Age at study start 3 mth (females 180 g) Number of animals: not explicitly stated for parental stock but 252 offspring subjected to further treatments and tests. Treatment: Ethanol was administered as a 12.5% v/v solution in distilled water by gavage to yield a dosage of 1 g/kg/day to dams throughout gestation alone or through gestation and

lactation.

Controls: Sucrose was added to distilled water vehicle to provide isocaloric control.

Mating conditions: Females were housed singly with male for 4 days.

Offspring were appropriately cross-fostered and divided into those that had not experienced exposure to ethanol, those that had experienced ethanol in utero and those that had experienced etanol exposure in utero and throughout lactation.

Dams were weighed during gestation. Offspring were weighed on days 3, 10, 20, 30, 45 and 63.

Offspring were subjected to assessments in Two-Way Active Avoidance (Shuttle-Box) Tests at 9 and 12 weeks and at 5 months.

Blood alcohol levels were determined on gestation day 14 and post natal day 14.

Remark

Statistical analysis was by ANOVA and Chi-squared analysis. This study is included as a neurotoxicity study in Chapter 5.9.

Result

Mortality was significantly increased (32% versus 7% in controls) in offspring exposed to ethanol during pregnancy with continued postnatal exposure having no significant further effect.

Offspring cross-fostered to dams that had been exposed to ethanol only during pregnancy showed even greater mortality (59%). Growth in offspring was delayed during the first 9 weeks. Learning was impaired in rats of both gender at 9 weeks relative to controls. This remained evident in males, but not females, at 5 months.

No visible malformations observed.

In offspring treated both pre- and post-natally with ethanol, 60% were poor learners compared with 33% in sucrose controls.

Blood ethanol levels were 35.0 +/- 5.8mg/100ml.

Conclusion

Ethanol at a dose of 1 g/kg/day administered to dam rats during

	gestation and lactation produce growth and behavioural changes in the offspring.
Reliability	(2) valid with restrictions Single dose used and no NOAEL established. High levels of mortality also a concern; high levels of cannibalism (possibly due to aggressive behaviour linked to alcohol withdrawal) offered as a possible explanation by authors.
Reference	Vaglenova, J., Petkov, V.V. (1998). Fetal alcohol effects in rats exposed pre- and postnatally to a low dose of ethanol. Alcohol: Clin and Exp Res 22 (3): 697-703.
12.11.2004	(304)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Mouse
Sex	Female
Strain	C57BL
Route of admin.	oral feed
Exposure period	
Frequency of treatm.	ad lib
Duration of test	
Doses	17%, 25% and 30% ethanol-derived calories
Control group	Yes
NOAEL maternal tox.	= 17 %
NOAEL teratogen.	= 17 %
LOAEL Maternal Toxicity	= 25%
LOAEL Teratogenicity	= 25%
Method	other
Year	1979
GLP	no data
Test substance	ethanol (64-17-5)
Remark	Age at study start 4-5 months Dosage: NOAEL and LOAEL doses given as % ethanol-derived calories. NOAEL (teratogenicity) effect is malformed foetuses and litter weight. Doses are calculated to be equivalent to 17, 29 and 28 g/kg bodyweight Ethanol or sucrose was added to provide calories. Number of animals per dose per sex: not explicitly stated but approximately 16. Mating conditions: Females were housed singly with proven studs until vaginal plugs were found. Dams were weighed on days 0, 4, 10 and 18 (at sacrifice). Foetuses were examined externally and internally for malformations;

implants and resorptions were recorded as was litter weight.
No maternal organs were examined and foetuses were examined for external and visceral malformations.
Statistical tests were t-tests or chi-square tests; p=<0.05 regarded sign.

Result

No mortality occurred.

Maternal data are not given for the following:

Number pregnant per dose level Number aborting Pre- and post-implantation losses Number of corporea lutea (Duration of pregnancy not relevant) Haematology and blood chemistry findings Gross pathology in dams Organ weight changes Histopathology incidence and severity.

Maternal data are given for the following:

The numbers of resorptions were one per litter at the two lower doses and 2/litter at the higher dose.
Number of implantations were 7.3/litter in all ethanol-treated groups.
Maternal weight gains were not affected by treatment.
Rates of diet consumption were 12.02 mild, 12.86 mild and 10.31 mild in the 3 ethanol dosed groups.
Clinical signs included slight tremulousness at the high-dose group when ethanol-containing diet was removed.

Blood alcohol levels ranged 3 mg% to 384 mg% across the 3 treatment groups.

Foetal data are not given for the following:

Litter size Number viable Sex ratio Postnatal growth Postnatal survival

Foetal data are given for the following:

Litter weights were not significantly affected by ethanol treatments.
Grossly visible abnormalities affected limb, eye, brain, heart, uro-genital tract and abdomen. Litter weight was not affected by ethanol-containing diets but malformations were significantly increased by maternal diets containing 25% or more of ethanol-derived calories.

	Grossly visible abnormalities, external, soft tissue and skeletal abnormalities affected the limb, eye, brain, heart, urogenital tract and abdomen of foetuses.
Conclusion	The teratogenicity of ethanol is demonstrated.
Reliability	(2) valid with restrictions Well reported study which established a NOAEL.
Reference	Randall, C. and Taylor, W. (1979) Prenatal ethanol exposure in mice: teratogenic effects. Teratol. 19: 305-312.
12.11.2004	(305)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	mouse
Sex	male
Strain	Swiss Webster
Route of admin.	oral feed
Exposure period	28 days
Frequency of treatm.	ad libitum
Duration of test	28 days
Doses	6.3% ethanol in liquid diet (32% ethanol-derived calories)
Control group	yes
NOAEL maternal tox.	< 32%
NOAEL teratogen.	< 32%
LOAEL Maternal Toxicity	= 32%
LOAEL Teratogenicity	= 32%
Method	other
Year	1981
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Age at study start: 190 days.
	Number of animals per group is not stated.
	Ethanol was added to diet and control diet contained an isocaloric amount of sucrose.
	Bodyweights were measured every two days. Blood samples were taken for blood alcohol levels.
	Mating: 48 h after ethanol or sucrose diets were removed males were mated with nulliparous females by 5-days cohabitation in the same cage. If no vaginal plugs were found, new females were offered. Mating lasted until 11 days after the last ethanol treatment.

	Only pregnancy rate and resorptions were recorded for dams. Corpora lutea were counted although data are not presented. Males were not examined. Foetal examination included crown-rump length, viability, ,. sex ratio, litter size and weight and grossly visible visceral and skeletal abnormalities.
Remark	These are PATERNAL NOAEL and LOAEL, not maternal. Fertilizaton rate was decreased 1/9 among matings 3-5 days after treatment.
Result	Crown rump length was reduced in the one litter produced by mating 3-5 days after paternal ethanol treatment. Nine females became pregnant per dose level. There were no abortions although pregnancy rates were reduced. Resorption rates varied 0-27% across mating intervals but were unaffecetd by ethanol treatment. Implantations, implantation losses and numbers of corpora lutea were not reported. Paternal bodyweights were unaffected by treatment. Clinical signs, haematological and blood biochemical parameters were not reported. Blood alcohol levels reached 296 +/- 19 mg%. Gross pathology, organ weight changes and histopathological incidences were not studied. Foetal changes: Litter size and weights. percentage of live foetuses and sex ratios were unaffecetd by ethanol treatment. Only 2 abnormalities (undescended testes and body asymmetry) occurred in 95 pups sired by treated males. Skeletons were not examined.
Conclusion	The role of paternal alcohol intake on anomalies seen in foetal alcohol syndrome was not conclusively established.
Reliability	(2) valid with restrictions Well reported study but only a single high dose used, which did not allow a no effect level to be established.
Reference	Randall, C. and Taylor, W. (1979) Prenatal ethanol exposure in mice: teratogenic effects. Teratol. 19: 305-312
12.11.2004	(305)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Mouse
Sex	Female

Strain	CBA
Route of admin.	oral feed
Exposure period	-31 to 17 gestation
Frequency of treatm.	ad libitum
Duration of test	
Doses	15, 20, 25 and 30% ethanol-derived calories
Control group	Yes
NOAEL maternal tox.	< 15%
NOAEL teratogen.	< 15%
LOAEL Maternal Toxicity	= 15%
LOAEL Teratogenicity	= 15%
Method	other
Year	1977
GLP	no data
Test substance	ethanol (64-17-5)
Remark	No early deaths were reported, No. pregnant per dose level: 8-10 All implants were resobed at the highest concentration of ethanol in diet. Resorption rates were 2% and 0% in controls and 57%, 72% and 100% in respective treatment groups. Numbers of implantations were 4.8 and 5.6 in controls and 4.0, 5.5, 5.2 and o in the treatment groups. Pre- and post-implantation losses were not specified. No. of corpora lutea were not counted. Clinical signs were not discussed although dams were described as 'alcoholic'. Blood alcohol levels before mating werer 0 and ° mg/dl in controls and 73, 121,174 and 315 mg/dl in treatment groups. Liver weight relative to body weight measured in 3 females per group before matlng were not affected by treatment and there were no histopathological effects seen in liver tissue.
Result	Foetal data: Litter size is not given. Foetal weights were depressed by treatment with means of 0.97 and 0.95 g in controls and 0.64, 0.33 and 0.51 g in the 3 lowest ethanol dose groups. Defects included skeletal abnormalities at 100% incidence in all 3 ethanol treated groups. These effects were primarily of the occipital bone but also affected the sternum and ribs. Visceral abnormalites affected 0% of foetuses in either control

	group and 36%, 100% and 100% of foetuses in the 3 ethanol treated groups. Dilated brain ventricles were the most frequent anomaly but open eyelids, exencephaly, gastroschisis and heart defects also occurred in the higher dose groups.
Test condition	Age at study start: 60-100 days. Number of animals per group: at least 8 per group.. Ethanol was added to diet and control diet contained an isocaloric amount of sucrose. Females received ethanol in diet for 10 days before dose graduated to next higher concentration until there were 10 females in each diet group.. Depending on dose group, animals received ethanol for 30 to 80 days before mating. Bodyweights were measured every two days. Blood samples were taken for blood alcohol levels. Mating: 48 h after ethanol or sucrose diets were removed males were mated with nulliparous females by 5-days cohabitation in the same cage. If no vaginal plugs were found, new females were offered. Mating lasted until 11 days after the last ethanol treatment. Only pregnancy rate and resorptions were recorded for dams. Corpora lutea were counted although data are not presented. Males were not examined. Foetal examination included crown-rump length, viability, sex ratio, litter size and weight and grossly visible visceral and skeletal abnormalities.
Reliability	(2) valid with restrictions Not a standard study protocol but appears to be well conducted and reported. Limited and very high dose does not allow a NOAEL to be established.
Reference	Chernoff, G. (1977). The fetal alcohol syndrome in mice: an animal model. Teratol. 15: 223-230.
12.11.2004	(307)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Mouse
Sex	Female
Strain	CD-1
Route of admin.	Gavage

Exposure period	8-14 gestation
Frequency of treatm.	once per day
Duration of test	
Doses	2,200, 3,600, 5,000 and 7800 mg/kg bw
Control group	Yes
NOAEL maternal tox.	= 2200 mg/kg bw
NOAEL teratogen.	>= 6400 mg/kg bw
LOAEL Maternal Toxicity	= 3600 mg/kg bw
LOAEL Teratogenicity	> 6400 mg/kg bw
Method	other
Year	1987
GLP	no data
Test substance	other TS: 200 proof ethanol (64-17-5)
Method	Age at start: 8-10 wks Number of animals per dose per sex: 6 confirmed pregnant/group. Ethanol was administered by gavage in distilled water in 10 ml bolus doses. . Clinical observations performed were physical examination and weight recording 6 times through pregnancy. Viability checked twice daily. Females were paired 1: 1 with males and vaginal plugs were indicative of pregnancy. Parameters assessed were maternal bodyweights, numbers of implantation sites, resorptions, live and dead foetuses, external abnormalities. No organs were examined at necropsy. Statistical tests were Bartlett's for homogeneity of variance, one-way ANOV A, Dunnett's, Duncan, Kruskal-Wallis, Dunn's and nested ANOV A.
Remark	Maternal data: Mortality and day of detah: No control animals died. Mortality rates in treated groups were 0/6, 1/6, 4/6, 5/6 and 6/6. Day of death not reported. Number pregnant per dose level: 6 Number aborting: Not reported. Possibly 2 litters were aborted at 5000 mg/kg. A surviving dam at 6400 mg/kg delivered a litter. Number of resorptions: Not distinguished. Resorptions per litter did not differ from control below 5000 mg/kg. Mean implantations ranged from 10.5 in controls to 13.83 but no significant difference noted. Pre- and post-implantation loss: Not reported.

No. of corpora lutea: Not measured.
Duration of pregnancy: dams killed on gestation day 18.
Bodyweight: Not affected by treatment.
Food consumption: not reported.
Clinical signs: Timing and duration not reported. At 3600 mg/kg and above

dams were lethargic with staggering gait and or laboured breathing.
Haematological findings: Not measured.
Clinical biochemistry: Not measured.
Gross pathology: Not reported.
Organ weight changes: Not measured.
Histopathology: Not reported.

Foetal data:

Litter size and weights: Not reported. Group means were not significantly different from controls.
Number viable: Mean number of dead foetuses per litter did not vary significantly with dose and ranged 0 to 0.5. Number of live foetuses per litter differed significantly from controls at 5000 mg/kg.
Sex ratio: Not reported.
Postnatal growth: Not applicable.
Postnatal survival: Not applicable.
Grossly viable abnormalities etc: No externally malformed foetuses were found in treated groups. Other types of abnormality were not sought.

Result

No maternal mortality occurred at 2200 mg/kg but 1/6 dams died at 3600 mg/kg rising to 6/6 at 7700 mg/kg. At doses of at least 3600 mg/kg, dams were lethargic and showed staggered gait and/or laboured breathing.

At 5000 mg/kg, resorption of litter were increased and live foetuses/litters were decreased. This was not apparent in the one litter at 6400 mg/kg. No other fetal effects were seen.

Foetal data:

Group mean litter weights ranged from l.33g (controls) to 0.99 g and did not vary with statistical significance. Mean number of dead foetuses per litter was not dose related and ranged from 0 to 0.5.

No externally visible malformations were found in foetuses

	from treated animals.
Conclusion	No dose-related adverse effects on foetuses were observed at doses close to those causing acute maternal toxicity.
Reliability	(2) valid with restrictions Well reported study but not to a standard protocol.
Reference	Wier, P., Lewis, S., Traul, K. (1987) A comparison of developmental toxicity evident at term to postnatal growth and survival using ethylene glycol monoethyl ether, ethylene glycol monobutyl ether and ethanol. Teratogen Carcinogen Mutagen 7: 55-64.
12.11.2004	(309)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	Female
Strain	Sprague-Dawley
Route of admin.	drinking water
Exposure period	Days 6-15 gestation
Frequency of treatm.	Daily
Duration of test	ad-libitum
Doses	15% ethanol in water
Control group	yes, concurrent vehicle
NOAEL teratogen.	>15 %
Result	not developmentally toxic
Method	other
Year	1978
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Animal details: supplied by Spartan Research Animals, Haslett, Michigan; weight 250-270 g Acclimation: 2-3 weeks at 72 deg F and 45% RH Light cycle 12 hr dark, 12 hr dark. Dosing: Liquid provided via a ball tipped waterer to minimise evaporation. Food: Purina lab chow. Day 0 taken when sperm observed in a vaginal smear. Blood alcohol determinations in non pregnant animals (using an alcohol dehydrogenase method): 10 am, 2 pm, 10 pm, 2 am and 6 am on day 4 of treatment. Sacrifice: day 21 Observations: -Weights (dams daily and offspring) - Live, dead and resorbed fetuses.

- Crown-rump length - Number of each sex - External examination and check for cleft palate.
- One third of fetuses examined histopathologically for soft tissue damage;
heads preserved in Bouins solution and examined for soft tissue damage but not skeletal alterations.
- All fetuses preserved in alcohol and subsequently processed for skeletal alterations.
Statistical evaluation: Litter used as experimental unit. Wilcoxon test as modified by Hasseman and Hoel to evaluate incidence of fetal alterations and resorptions. Analysis of variance used for maternal and fetal bodyweights. Level of significance $p<0.05$.

Result

Mean consumption of food and liquid by rats given ethanol was significantly less that that of control rats during the experimental period. As a result, mean gain in body weight of the exposed rats was also significantly less between days 6 and 16 of gestation. Ethanol ingestion did not affect fetal survival adversely, but mean fetal body weight was significantly less than that of the control litters.

No malformed fetuses were found in the experimental litters. No external or soft tissue alterations were observed among the fetuses of the control or experimental litters. Skeletal malformations were not detected in the experimental group but skeletal variants consisting of unfused bones of the skull and cervical vertebra with missing centra occurred in the ethanol litters at an incidence significantly greater than in the control litters.

Reduced fetal body weight (5.41g+/-0.25; control 5.70+/-0.35)
Non fused sternebrae (100 in 18 litters; control 45 in 8)
Vertebrae-missing centra (117 in 18 litters; control 15 in 8)
Wavy ribs (13 in 5 litters; control 3 in 3)
Note: total skeletal fetuses examined 223 in 29 litters

Overall there were no definite teratogenic abnormalities.

Peak blood alcohol levels: 40 mg/100ml blood at 6am.

Test substance

Reagent grade ethyl alcohol 190 proof from US Industrial Chemicals Co.

Reliability

(2) valid with restrictions
Well reported study but only single dose used.

Reference

Schwetz, B.A., Smith, FA, Staples, R.E. Teratogenic potential of ethanol in mice, rats and rabbits. Teratology 1978; 18: 385-

	392.
12.11.2004	(310)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Mouse
Sex	Female
Strain	CD-1
Route of admin.	drinking water
Exposure period	days 6-15 of gestation
Frequency of treatm.	Daily
Duration of test	ad libitum
Doses	15% ethanol in drinking water
Control group	yes, concurrent vehicle
NOAEL teratogen.	> 15 %
Result	
Method	no developmental toxicity observed.
Year	other
GLP	
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Animals: Virgin mice from Carworth Animals, Portage, Michigan, weight 2225g. Acclimation: 2-3 weeks at 72 deg F and 45% RH; light cycle 12 hr dark, 12 hr dark. Dosing method: Liquid provided via a ball tipped waterer to minimise evaporation. Food: Purina lab chow. Day 0 taken when vaginal plug observed in mice. Blood alcohol determinations in non pregnant animals (using an alcohol dehydrogenase method): 10 am, 2 pm, 10 pm, 2 am and 6 am on day 4 of treatment. Sacrifice: day 18 Observations: -Weights (dams daily and offspring) - Live, dead and resorbed fetuses. - Crown-rump length - Number of each sex - External examination and check for cleft palate. - One third of fetuses examined histopathologically for soft tissue damage; heads preserved in Bouins solution and examined for soft tissue damage but not skeletal alterations. ~ All fetuses preserved in alcohol and subsequently processed for skeletal alterations. Statistical evaluation: Litter used as experimental unit. Wilcoxon test as modified by Hasseman and Hoel to evaluate

	incidence of fetal alterations and resorptions. Analysis of variance used for matemal and fetar;t~ bodyweights. level of
Result	significance p<0.05. Mice receiving ethanol consumed significantly less food and liquid than control mice. Consumption returned to control levels within two days after removal of the ethanol. Maternal body weight gain reflected the decreased consumption of food and liquid. The number of Jive fetuses/litter was not significantly affected but fetal weight and length were significantly decreased upon comparison to control values. Other than one fetus with cleft palate and two fetuses from different litters that had exencephaly with open eye, no external or soft tissue alterations were noted among the offspring of dams given ethanol. The incidence of exencephaly, open eye, and cleft palate did not differ significantly from control values. Skeletal malformations were not detected but the incidence of several minor skeletal variants e.g. delayed ossification of the centra of cervical vertebra, non-fused sternebrae and delayed ossification of sternebrae (less than 90% ossified), was significantly increased among the litters of mice ingesting ethanol. Significant effects in mice: reduced fetal body weight (0.95g+/-0.12; control 1.11+/-0.11) Reduced crown rump length (22.2+/-1.0mm; control 23.5+/-1.2mm) Non fused sternebrae (52 in 18 litters; control 26 in 12) Delayed ossification (59 in 17 litters; control 7 in 4) Note: total skeletal fetuses examined 239 in 21 litters
Test substance	
	Overall there were no significant teratogenic abnormalities. Peak blood alcohol levels were 204 mg/100ml at 2am. Reagent grade ethyl alcohol 190 proof from US Industrial
Reliability	Chemicals Co. (2) valid with restrictions Well reported study but only single dose level used.
Reference	Schwetz, BA, Smith, FA, Staples, R.E. Teratogenic potential of ethanol in mice, rats and rabbits. Teratology 1978; 18: 385-392.
12.11.2004	(311)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rabbit
Sex	Female
Strain	New Zealand white
Route of admin.	drinking water

Exposure period	Days 6-18 of gestation
Frequency of treatm.	Daily
Duration of test	ad libitum
Doses	15% ethanol in drinking water
Control group	yes, concurrent vehicle
NOAEL teratogen.	>15 %
Result	not developmentally toxic
Method	other
Year	
GLP	no data
Test substance	ethanol (64-17-5)
Method	Animals: supplied by Langshaws Rabbitry, Augusta, Michigan. Initial animal weights not specified. Acclimation: 2-3 weeks at 72 deg F and 45% RH; light cycle 12 hr dark, 12 hr dark. Dosing: Liquid provided via a ball tipped waterer to minimise evaporation. Food: Purina lab chow. Day 0 taken when mating observed. Blood alcohol determinations in non pregnant animals (using an alcohol dehydrogenase method): 10 am, 2 pm, 10 pm, 2 am and 6 am on day 4 of treatment. Sacrifice: day 29 Observations: -Weights (dams daily and offspring) - Live, dead and resorbed fetuses. - Crown-rump length - Number of each sex - External examination and check for cleft palate. - One third of fetuses examined histopathologically for soft tissue damage; heads preserved in Bouins solution and examined for soft tissue damage but not skeletal alterations. - All fetuses preserved in alcohol and subsequently processed for skeletal alterations. Statistical evaluation: Litter used as experimental unit. Wilcoxon test as modified by Hasseman and Hoel to evaluate incidence of fetal alterations and resorptions. Analysis of variance used for maternal and fetal bodyweights. Level of significance $p<0.05$.
Result	Liquid consumption of animals receiving ethanol was significantly less than that of controls as was mean body weight (latter difference as statistically significant on days 12 and 18 of gestation.) The incidence of resorptions among litters of rabbits given ethanol was approximately twice that observed in the

	control litters; this increase was due primarily to the complete resorption of two litters in the ethanol group. Fetal body measurements and the number of malformed fetuses were comparable between the control and experimental litters. No alterations were observed at an incidence that was significantly increased in the ethanol group compared to the control group. Minor vascular alterations observed have all been found to occur spontaneously in control groups of this strain of rabbit. Overall there were no teratogenic abnormalities Peak blood alcohol level was 24mg/100ml at 6am.
Test substance	Reagent grade ethyl alcohol 190 proof from US Industrial Chemicals Co.
Reliability	(2) valid with restrictions A well reported study but only a single dose used.
Reference	Schwetz, B.A., Smith, FA, Staples, R.E. Teratogenic potential of ethanol in mice, rats and rabbits. Teratology 1978; 18: 385-392.
12.11.2004	(311)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	male/female
Strain	Sprague-Dawley
Route of admin.	inhalation
Exposure period	7 hours
Frequency of treatm.	Daily
Duration of test	see method details
Doses	0, 10000, 16000 ppm
Control group	Yes
NOAEL maternal tox.	> 16000 ppm
Other NOAEL: behavioural/teratogenicity	> 16000 ppm
Other NOAEL: fertility	> 16000 ppm
Result	Negative
Method	other: see method details
Year	1985
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Behavioural testing procedures:

Behavioral testing was from days 10- 90. Female and male pups were selected randomly. For each test, one female and one male were used from each litter. Testers were not aware of the treatment groups to which subjects belonged. Tests used:
1. Rotorod, 9 cm in diameter and 10 cm long, and the surface was rough with sand. Rotation speed increased until the animals had five unsuccessful trials.
2. The open field was 1 m in diameter, with an enclosure wall 0.5 m high.
Animals were tested for 3 min.
3. Optical digital animal activity monitor. The animal test area was a 40x40x20 cm Plexiglas cage which had 30 photodiodes per side. Activity scores were summed over the 3 days of testing at each age.
4. Running wheel activity over a 24 hr period, separated into day and night activity scores.
5. Two shuttle boxes in sound-attenuated chambers, with 4 cm center partitions. Metal grid floors to which electrical shocks could be applied. 5 sec warning stimulus.
hr/day until they no longer responded sufficiently to receive reinforcement.

Exposure was conducted in $0.5m^3$ chambers with dynamic air flow (one air change per minute.)

Animals: 18/group. Starting weights 400-500g.
Temperature: 73 +/- 3F. Humidity: average 40-50%.
Exposure period: Males: 6 weeks; 2 day non exposure period before mating. Females: GD 1-20. Mating period 5 days. 7 hours per day.
Mating confirmed by presence of sperm plugs under cages or vaginal smears. Females housed individually.
Analytical monitoring: Yes (IR analyser - exposures found to be within 11 % of nominal). Independently cross-checked with charcoal adsorption tubes.
Parameters measured: weights (daily), food and water intake as measures of maternal toxicity.
Parturition: All litters culled to 4 pups of each sex and fostered to untreated dams which had delivered within past 2 days. On PND10 pups individually identified by ear punch and randomly assigned to behavioural study
groups.

Result

No effect on weight gain. feed or water intake. No effect on fertility or litter sizes.
Behavioural testing showed no difference from controls in any of the behavioural tests.

	Previous studies quoted as showing exposures to 10000 and 16000 ppm ethanol typically give rise to blood ethanol concentrations of 30 and 500 mg/l ethanol. Authors calculate that for rats exposures in excess of 11000 ppm are required to begin accumulating ethanol in the blood and that ethanol is no more toxic by the inhalation route than by other routes.
Reliability	(2) valid with restrictions Well reported study but not to a standard protocol. Route of exposure highly relevant.
Reference	Nelson BK, Brightwell WS, Mackenzie-Taylor DR, Burg JR, Massari VJ (1988) Neurochemical but not behavioral deviations in the offspring of rats following prenatal or paternal inhalation exposure to ethanol. Neurotoxicol Teratol 10, 15-22. Nelson BK; Brightwell, WS, Burg JR (1985) Comparison of Behavioural Teratogenic Effects of Ethanol and n-propanol administered by inhalation to rats. Neurobehav Toxicol Teratol 7, 779-83.
12.11.2004	(291) (292)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	male/female
Strain	Sprague-Dawley
Route of admin.	inhalation
Exposure period	7 hours
Frequency of treatm.	Daily
Duration of test	see method details
Doses	0, 10000, 16000 ppm
Control group	Yes
NOAEL teratogen.	
Result	
Method	other: see method details
Year	1988
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Behavioural testing procedures: Behavioral testing was from days 10 - 90. Female and male pups were selected randomly. For each test, one female and one male were used from each litter. Testers were not aware of the treatment groups to which subjects belonged. Tests used: 1. Rotorod, 9cm in diameter and 10 cm long, and the surface was rough with sand. Rotation speed increased until the animals

had five unsuccessful trials.
2. The open field was 1 m in diameter, with an enclosure wall 0.5 m high.
Animals were tested for 3 min.
3. Optical digital animal activity monitor. The animal test area was a 40x40x20 cm Plexiglas cage which had 30 photodiodes per side. Activity scores were summed over the 3 days of testing at each age.
4. Running wheel activity over a 24 hr period, separated into day and night activity scores.
5. Two shuttle boxes in sound-attenuated chambers, with 4 cm center partitions. Metal grid floors to which electrical shocks could be applied. 5 see warning stimulus.
hr/day until they no longer responded sufficiently to receive reinforcement.
Exposure was conducted in 0.5m3 chambers with dynamic air flow (one air change per minute.) Dosing method described in detail.

Animals: Starting weights: females, 15 per group, 176-200g; males, 18 per group >390g.
Temperature: 24+/-2C. Humidity: -40%. 12hr light/dark cycle.
Exposure period: Males: 6 weeks; 2 day non exposure period before mating. Females: GD 1-20. Mating (1:1 male:female) period 5 days. Mating confirmed by presence of sperm plugs under cages or vaginal smears. Females housed individually. Stock males used as sires for controls.
Analytical monitoring: Yes (IR analyser - exposures found to be +/-200ppm of nominal). Independently cross-checked with charcoal adsorption tubes
analysed by gas chromatography.
Parameters measured weekly: weights food and water intake as measures of maternal toxicity.
Parturition: All Jitters weighed within 16 hrs. Litters less than 3 pups per sex discarded. Offspring weighed on PND 7 and checked for abnormalities Neurochemical analysis: One female and one male (untested) from 5 litters sacrificed PND 21 for analysis of concentrations of protein and the neurotransmitters acetylcholine. dopamine, norepinephrine, 5hydroxytryptamine, substance P. beta-endorphin, and Met-enkephalin. Pup brains were separated into the four general brain regions of cerebrum, cerebellum, brainstem meduila-pons), and midbrain and frozen until assayed by sonic homogenization in 8 ml of O. 1 N He!.

Statistical Analyses: Behavioral data were analyzed using multivariate analysis of variance or an m-ranking procedure.

	Repeated measures analyses were conducted where appropriate to p<O.05. Neurochemical data were analyzed using Analysis of Variance followed by Duncan's Multiple Range post-hoc tests where a significance was found.
Remark	Authors concluded that industrial inhalation exposure to ethanol may not be expected to produce alarming blood ethanol levels and that inhalation exposures to ethanol which produce narcosis in maternal rats are not teratogenic.
Result	Males: weight gain retarded during 1st week but normal thereafter. Females: no effect on weight gain. Feed intake retarded during 1st week but normal thereafter at 16000ppm. No effects on litter size, still births, length of pregnancy, offspring survival. . No effect observed in behavioural study tests. No effect on dopamine, substance P, beta-endorphin and acetylcholine levels. Significant effects on norepinephrine, 5-hydroxytryptamine but magnitude and direction of changes not correlated with dose. Level of Met-enkephalin affected at lower but not higher dose.
Reliability	(2) valid with restrictions Well reported study but not to a standard protocol. Route of exposure highly relevant.
Reference	Nelson BK, Brightwell WS, Mackenzie-Taylor DR, Burg JR, Massari VJ (1988) Neurochemical but not behavioral deviations in the offspring of rats following prenatal or paternal inhalation exposure to ethanol. Neurotoxicol T eratol 10, 15-22.
12.11.2004	(291)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Monkey
Sex	
Strain	Macaca Fascicularis
Route of admin.	other: in utero expusure
Exposure period	throughout gestation
Frequency of treatm.	Daily
Method	other
Year	1999
GLP	no data
Test substance	ethanol (64-17-5)
Remark	There was some correlation with cognitive performance and this study is further considered in Neurotoxicity.
Result	Standardised craniofacial cephalograms of 18 macaques

	exposed weekly to ethanol or sucrose solution in utero were measured at ages 1, 6, 12 and 24 mths showed that there may be a critical period for induction of alcohol induced craniofacial alterations. These were most prominent at 6 mths and diminished thereafter as underlying changes in skeletal structure caused disappearance of the thin upper lip and smooth philtrum characteristic of fetal alcohol syndrome.
Reliability	(4) not assignable
Reference	Astley, S.J., Magnuson, S.I., Omnell, L.M., Clarren, SK Fetal Alcohol Syndrome: Changes in craniofacial form with age, cognition, and timing of ethanol exposure in the macaque. Teratology 1999; 59: 163-172.
12.11.2004	(312)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Human
Sex	
Strain	
Route of admin.	oral feed
Method	other: literature review 1999
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	The large and growing evidence of the effects of parental alcohol consumption on offspring was assessed. Study of clinical cases support the conclusion that chronic heavy maternal drinking consistent with alcohol dependence or alcoholism is an aetiological factor in foetal alcohol syndrome.. The effects of this can extend beyond puberty with cognitive and neurobehavioural problems continuing and with the most deleterious of outcomes. Animal studies have demonstrated a dosage relationship in the absence of the confounding factors prevalent in humans (e.g. poor maternal health and tobacco smoke) and that the effects of alcohol are most pronounced on the brain. Individual differences in maternal metabolism and genetic factors may explain why the infants of some problem-drinking mothers are more affected than others but there is also some evidence of a threshold of drinking below which adverse effects cannot be detected. This may be around 30 to 40 g per day (4-5 UK drinks or 2.5 to 3.5 US drinks per day). This level is well above the levels defined as moderate drinking for non-pregnant women.
Reliability	This is a literature review presented as a book chapter. (4) not assignable
Reference	Plant, M.L., Abel, E.L., Guerri, C. (1999). Chapter 6: Alcohol and Pregnancy. In: Health Issues Related to Alcohol

	Consumption. Ed. Macdonald, I. International Life Sciences Inst. 2nd edition. ISBN 1-57881-062-0.
12.11.2004	(313)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	Female
Strain	
Route of admin.	drinking water
Exposure period	4 weeks and throughout gestation
Frequency of treatm.	
Duration of test	
Doses	20% alcohol before mating and 30% through gestation; 3500 mg/kg/day throughout treatment.
Control group	
NOAEL teratogen.	
Result	
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Offspring of female Sprague-Dawley rats that were administered ethanol in water as the drinking fluid at a concentration of 20% v/v for four weeks before mating and at a concentration of 30% v/v during gestation were physically and developmentally retarded and failed to catch up with control offspring during the first four weeks postpartum.
Reliability	(4) not assignable
Reference	Leichter, J. and Lee, M. Effect of maternal ethanol administration on physical growth of the offspring of rats. Growth 1979; 43: 288-297.
12.11.2004	(314)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	Female
Strain	Sprague-Dawley
Route of admin.	drinking water
Exposure period	4 weeks before mating and on days 1 to 20 of gestation.
Frequency of treatm.	
Duration of test	
Doses	20-30% in water; estimated 4000 mg/kg/day.

Control group	no data specified
NOAEL teratogen.	
Result	
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	The offspring of Sprague-Dawley rats given 20% ethanol in the drinking water four weeks before mating and 30% ethanol in drinking-water until gestation day 20 had retarded skeletal development and decreased body weight but no gross malformation.
Reliability	(4) not assignable
Reference	Lee, M., Leichter, J. Skeletal development of foetuses of rats consuming alcohol during gestation. Growth 1983 ;47: 254-262.
12.11.2004	(315)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	Female
Strain	Long-Evans
Route of admin.	drinking water
Exposure period	10 or 90 days before gestation and during gestation
Frequency of treatm.	
Duration of test	
Doses	9220 mg/kg/day during 10 day pre-exposure; 14500 mg/kg/day in 90 day pre-exposure and 11,300 mg/kg/day during gestation
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	This is an important study in that it confirms that 5% v/v in feed delivers a dosage of 12,000 to 14,000 mg/kg.
Result	A decrease in foetal bodyweight was noted in each dosage regimen. There were no gross abnormalities or skeletal defects noted.
Reliability	(4) not assignable
Reference	Samson, H .H. Maternal ethanol consumption and fetal development in the rat: a comparison of ethanol exposure

	techniques. Alcohol Clin Exp Res 1981: 5: 67-74.
12.11.2004	(316)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	Long-Evans
Route of admin.	drinking water
Exposure period	GD 7 to delivery
Frequency of treatm.	
Duration of test	
Doses	10%
Control group	
Remark	Study was designed to assess ethanol effects on sexual differentiation.
Result	Gestation was prolonged and offspring of each sex showed decreased anogenital distances at birth. Pups nursed by ethanol-drinking mothers had a significantly earlier preputial separation, but there was no effect on adult masculine sex behaviour, plasma testosterone or weights of accessory sex glands.
Reliability	(4) not assignable
Reference	Chen J.J. & Smith E.R. 1979. Horm. Behav. 13, 219.
12.11.2004	(317)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Mouse
Sex	Female
Strain	other: not specified
Route of admin.	drinking water
Exposure period	from 11 weeks before mating and throughout gestation
Frequency of treatm.	
Duration of test	
Doses	10-20% in drinking water; Estimated 3000 to 5000 mg/kg/day
Control group	no data specified
NOAEL teratogen.	
Result	
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Retardation of muscle growth was seen in offspring killed at 12 weeks of age of inbred mice given 10-20% ethanol in the

	drinking-water for 11 weeks before mating and 30% ethanol after breeding until delivery. Prenatally, there was suppression of hyperplasia of muscle fibres during myogenesis; postnatally, there was suppression of normal hypertrophy of individual muscle fibres.
Reliability	(4) not assignable
Reference	Ihemelandu, E.C. Effect of maternal ethanol consumption on pre- and post-natal muscle development in mice. Growth 1984; 48: 35-43.
12.11.2004	(318)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Mouse
Sex	Female
Strain	C57BL
Route of admin.	drinking water
Exposure period	Before mating, throughout gestation and lactation
Frequency of treatm.	
Duration of test	as above
Doses	10% (v/v)
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Fetotoxicity and structural teratology: When female C57BI/Crgl mice were given 10% ethanol (v/v) in water as the drinking fluid before mating, throughout gestation and lactation, no significant effect on pup development or behaviour was seen.
Reliability	(4) not assignable
Reference	Thiessen, D.O., Whitworth, N.S., Rodgers, O.A. Reproductive variables and alcohol consumption of the C57BI/Crgi female mouse. Q J Stud Alcohol 1966; 27: 591-595.
12.11.2004	(303)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Dog
Sex	Female
Strain	Beagle
Route of admin.	Gavage
Exposure period	

Frequency of treatm.	twice daily throughout gestation
Duration of test	
Doses	1800 mg/kg/day
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Dogs were administered 1.8 g/kg bw ethanol as a 25% solution by gavage twice daily and were given either a normal-protein or low-protein diet throughout gestation.
Result	Ethanol consumption and low dietary protein intake, independently of each other, significantly decreased maternal weight gain as well as the weight of the neonates.
Reliability	(4) not assignable
Reference	Switzer, B.R., Anderson, J.J.B., Pick, J.R. Effects of dietary protein and ethanol intake of pregnant Beagles fed purified diets. J. Nutr. 1986; 116: 689-697.
12.11.2004	(319)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Dog
Sex	
Strain	
Route of admin.	Gavage
Exposure period	throughout gestation
Frequency of treatm.	
Duration of test	
Doses	3 or 3.6 g/kg bodyweight
Test substance	ethanol (64-17-5)
Result	There were no gross or histological abnormality, a slight decrease in the number of offspring per litter and in pup weight, and an increase in the number of still births. Blood ethanol concentrations were 1.3-1.75 g/l.
Reliability	(4) not assignable
Reference	Ellis FW. et al. 1977. Fed. Proc. 36, 285.
12.11.2004	(320)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Monkey
Sex	Female
Strain	Macaca Fascicularis

Route of admin.	Gavage
Exposure period	Starting before day 10 or on day 40 of gestation
Frequency of treatm.	once per week throughout gestation as above
Duration of test	
Doses	0.3 - 4.1 g/kg bw
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Spontaneous abortion frequency increased at peak plasma ethanol concentrations above 2 g/1. Developmental alterations were observed consistently in offspring of monkeys with blood levels greater than 1.5 g/l when treatment was initiated at the start of gestation; infants exposed only after gestation day 40 were less consistently abnormal despite higher maternal blood ethanol levels (5.5g/I). There were developmental alterations and an increase in spontaneous abortions at peak plasma ethanol levels above 200 mg/100 mL Developmental alterations in offspring were consistent at blood alcohol levels in excess of 150 mg/100 ml.
Reliability	(4) not assignable
Reference	Clarren SK et al. 1987b. Teratology 35. 66A.
	Clarren, SK, Astley, S.J., Bowden, D.M. Pregnancy outcomesafter weekly oral administration of ethanol during gestation in the Pig-tailed Macaque (Macaca namestrina). Teratology 1987; 35: 345-354.
12.11.2004	(321) (322)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	male/female
Strain	
Route of admin.	oral feed
Exposure period	from 6 weeks before mating
Frequency of treatm.	
Duration of test	
Doses	Estimated much greater than 12,000 mg/kg/day
Control group	no data specified .
Method	other
Year	
GLP	no data

Test substance	95 – 99.9% ethanol (64-17-5)
Method	Male Sprague-Dawley rats maintained for six weeks on a liquid diet containing 10% ethanol were paired with untreated females.
Result	There was body weight loss and central nervous system impairment. and only half of the treated animals had successful matings, compared to all of the controls. There was a decrease in litter size and an increase in prenatal mortality among the litters.
Reliability	(4) not assignable
Reference	Klassen, R.W., Perdsaud, T,V.N. Experimental studies on the influence of male alcoholism on pregnancy and progeny. Exp. Pathol. 1976; 12: 38-45.
12.11.2004	(323)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	Female
Strain	Long-Evans
Route of admin.	oral feed
Exposure period	Days 6-20 gestation
Frequency of treatm.	
Duration of test	
Doses	35% of calorie intake, estimated 12,150 mg/kg/day
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Offspring showed lower maximal suckling pressure as well as suckling pattern changes.
Reliability	(4) not assignable
Reference	Rockwood, GA, Riuley, E.P. Suckling deficits in rat pups exposed to alcohol in utero. Teratology 1986; 33:145-151.
12.11.2004	(326)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	Female
Strain	Long-Evans
Route of admin.	oral feed

Exposure period	Days 6-20 of gestation
Frequency of treatm.	
Duration of test	
Doses	35% of calorie intake. Estimated 12,150 mg/kg/day.
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Males showed feminization; females showed masculinization indicating prenatal hormonal disruption.
Reliability	(4) not assignable
Reference	Meyer, L.S., Riley, E.P. Social play in juvenile rats prenatally exposed to alcohol.Teratology 1986; 34: 1-7.
12.11.2004	(327)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	Female
Strain	Wistar
Route of admin.	oral feed
Exposure period	From day 12 of gestation to 10 days post partum
Frequency of treatm.	
Duration of test	
Doses	Estimated 12,150 mg/kg/day; 36% of calorie intake.
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Offspring showed decreased ano-genital distance; decreased male reproductive organ weights 55 and 110 days post partum; lowered sex hormones (lH and testosterone), sexual motivation and performance; lowered phenotypic masculinization.
Reliability	(4) not assignable
Reference	Udani, M., Parker, S., Gavaler, J.S., Van Thiel, D.H. Effects of the in utero exposure to alcohol upon male rats. Alcoholism: Clinical and Experimental Research 1985; 9(4): 355-359.
12.11.2004	(328)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	Female
Strain	
Route of admin.	oral feed
Exposure period	16 weeks
Frequency of treatm.	
Duration of test	16 weeks
Doses	5% ethanol in liquid feed
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Mating of female Holtzman rats fed a liquid diet containing 5% ethanol for 16 weeks with untreated males resulted in no adverse effect on litter size or neonatal body weight.
Reliability	(4) not assignable
Reference	Krueger, W.A., Bo, W.J., Rudeen, P.K. Female reproduction during chronic ethanol consumption in rats. Pharmacal Biochem Behav 1982; 17: 629-631.
12.11.2004	(285)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	Female
Strain	Wistar
Route of admin.	oral feed
Exposure period	Before mating, throughout gestation and lactation
Frequency of treatm.	
Duration of test	as above
Doses	12% ethanol in sucrose solution (20-25% calorie intake)
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	When female Wistar rats were given 20-25% of the calories consumed as 12% ethanol in a sucrose solution as the drinking fluid before mating and throughout gestation and lactation, there was no effect on development of offspring There was no effect

	on development or offspring.
Reliability	(4) not assignable
Reference	Oisund, J.F., Fjorden. A-E.. Moerland, J. Is moderate ethanol consumption teratogenic in the rat? Acta Pharmacal Toxicol. 1976; 43: 145-155.
12.11.2004	(329)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	Female
Strain	
Route of admin.	oral feed
Exposure period	1 year
Frequency of treatm.	Daily
Duration of test	
Doses	Blood alcohol level of 22.8 mmol/l
Control group	yes, concurrent no treatment
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	To study the severity and degree of in utero alcohol effects in relation to the rate of maternal alcohol damage, multiparous i-year alcohol-fed rats were used, with an appropriate pair-fed control group. During pregnancy, alcoholic dams showed relatively high acetaldehyde levels (41 +/- 19 mumol/I) and blood alcohol levels of 22.8 +1- 14 mmol/1.
Remark	The stage of maternal alcohol illness, as indicated mainly by the extent of liver damage, may play an important role in the frequency and severity of in utero alcohol effects in the rat.
Result	Dams showed marked histological alterations in liver as well as high serum aspartate-aminotransferase, alanine-aminotransferase, alkaline phosphatase, glutamate dehydrogenase, and gamma-glutamyltransferase activities. The increase in serum enzyme levels did not correlate with an increase in hepatic enzyme levels since only glutamate dehydrogenase was enhanced in liver after 1 year of alcohol intake. In addition, except for an increase in low Km aldehyde dehydrogenase activity, there were no changes in liver alcohol metabolizing enzymes in chronic alcohol vs. pair fed females. Alcoholic rats showed a high incidence of damage in their progeny (resorptions, immature fetuses, decrease in fetal

	weight, etc.), and rats with the highest serum levels of theabove enzymes (especially glutamate dehydrogenase and gamma-glutamyl transferase) had severely affected progeny. Rats with minimal histological liver damage, in contrast, did not show resorptions.
Reliability	(4) not assignable
Reference	Sanchis, R., Sancho-Tello, M., Chirivella, M., Guerri, C. The role of maternal alcohol damage on ethanol teratogenicity in the rat Teratology 1987; 36(2):199-208.
12.11.2004	(330)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	Sprague-Dawley
Route of admin.	oral feed
Exposure period	GD 7 to parturition
Frequency of treatm.	
Duration of test	
Doses	liquid diet containing ethanol as 35% of calories
Test substance	ethanol (64-17-5)
Result	Absence of sexual dimorphism (saccharin preference and maze learning) was seen among offspring, suggesting disrupted perinatal androgen status.
Reliability	(4) not assignable
Reference	McGivern R.F. et al.1984. Science 224, 896.
12.11.2004	(331)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	Long-Evans
Route of admin.	oral feed
Exposure period	GD 6-20
Frequency of treatm.	
Duration of test	
Doses	liquid diet containing 35% ethanol derived calories
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Offspring males showed feminized behaviour and females showed masculinized behaviour, suggesting disruption of the hormonal environment prenatally.
Reliability	(4) not assignable

Reference	Meyer L.S. & Riley E.P. 1986. Teratology 34, 1.
12.11.2004	(332)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	Long-Evans
Route of admin.	oral feed
Exposure period	GD 6-20
Frequency of treatm.	
Duration of test	
Doses	liquid diet containing 35% ethanol derived calories
Test substance	ethanol (64-17-5)
Result	There was evidence of behavioural deficits, which persisted until adulthood. Female offspring showed a variety of deficits in maternal behaviour when adult, which may have been related to prenatal hormonal alterations.
Reliability	(4) not assignable
Reference	Barron S. & Riley E.P. 1985. Alcohol. Clin. Exp. Res. 9, 360.
12.11.2004	(333)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Mouse
Sex	Female
Strain	C3H
Route of admin.	oral feed
Exposure period	Days 0-17 of gestation
Frequency of treatm.	
Duration of test	Days 0-17 gestation
Doses	4.1 % w/v in liquid diet
Control group	no data specified
Method	other
Year	
GLP	no data as
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Groups of C3H mice were given a liquid diet or a fortified liquid diet, each either alone or with 4.1 % wlv ethanol, from days 0-17 of pregnancy; a further group was given an amount of liquid diet equal to that consumed by the group given liquid diet plus ethanol.

Result	Ethanol consumption inhibited foetal growth and development but did not affect litter size irrespective of the diet used.
Reliability	(4) not assignable
Reference	Goad, P.T., et al. The role of maternal diet in the developmental toxicology of ethanol. Toxicol Appl Pharmacol 1984; 73: 256-267.
12.11.2004	(334)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	
Sex	Mouse Female other: RAP Lv.
Strain	
Route of admin.	once on day 3 or 4 of gestation
Exposure period	
Frequency of treatm.	not specified no data specified other
Duration of test	
Doses	95 – 99.9% ethanol (64-17-5)
Control group	
Method	Preimplantation effects in a study on the effects of preimplantation exposure: mice were given ethanol intravenously on days 3 and 4 of pregnancy and offspring were examined on day 19 of pregnancy.
Result	On day 19 of gestation the mean foetal and placental weights were significantly lowered but there was no effect on skeletal development.
Reliability	(4) not assignable
Reference	Checiu, M. and Sandor, S. The effect of ethanol upon early development in mice and rats. IX. Late effect of acute. pre-implantation intoxication in mice. Morphol Embryol. 1986; 32: 511.
12.11.2004	(335)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Monkey
Sex	Female
Strain	other: rhesus and cynomolgus
Route of admin.	i.v.
Exposure period	1-2 minutes
Frequency of treatm.	
Duration of test	Gestation days 120-147
Doses	3 g/kg bodyweight
Test substance	ethanol (64-17-5)
Result	In monkeys given 3g/kg bw ethanol intravenously over 1-2 min

	on gestation days 120-147, transient but marked collapse of umbilical vasculature was observed within 15 min. This resulted in severe hypoxia and acidosis in the fetus, but recovery occurred during the succeeding hour.
Reliability	(4) not assignable
Reference	Mukherjee A.B. & Hodgen G.D. 1982. Science 218, 700.
12.11.2004	(336)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	Long-Evans
Route of admin.	oral unspecified GD 6 - 20
Doses	liquid diets containing ethanol (35% of total calories)
Test substance	ethanol (64-17-5)
Result	Offspring exerted a lower maximal suckling pressure, spent less time suckling during test sessions and displayed an altered suckling pattern.
Reliability	(4) not assignable
Reference	Rockwood GA& Riley E.P. 1986. Teratology 33, 145.
12.11.2004	(337)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	Female
Strain	Long-Evans
Route of admin.	oral unspecified
Exposure period	throughout gestation
Frequency of treatm.	
Duration of test	throughout gestation
Doses	1 or 2 g/kg bodyweight given daily
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Litter size, litter weight and mean pup weight were lowered but there were no gross malformations or behavioural teratogenic effects.
Reliability	(4) not assignable
Reference	Abel, E.L. Effect of ethanol on pregnant rats and their

	offspring. Psychopharmacology 1978; 57: 5-11.
12.11.2004	(338)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	Female
Strain	Long-Evans
Route of admin.	oral unspecified
Exposure period	Days 5-19 of gestation
Frequency of treatm.	
Duration of test	as above
Doses	6000 mg/kg achieving blood alcohol level of 260 mg/100 ml
Control group	no data specified other
Method	
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	Long-Evans rats administered 6 g/kg bw ethanol orally on gestation days 519 had blood ethanol concentrations of over 2.6 g/l. Fetuses had decreased body weight, increased body water and sodium content and decreased lipid-free solid content.
Reliability	(4) not assignable
Reference	Abel, EL, Greizerstein, H.B..Ethanol-induced prenatal growth deficiency: Changes in fetal body composition. J Pharmacol Exp Ther 1979;211 :668-671.
12.11.2004	(339)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	Female
Strain	Sprague-Dawley
Route of admin.	oral unspecified
Exposure period	Days 1-21 of gestation
Frequency of treatm.	
Duration of test	as above
Doses	36% of calorie intake achieving blood alcohol levels of 150-200 mg/100 ml
Control group	no data specified
Method	other
Year	
GLP	no data
	95 – 99.9% ethanol (64-17-5)

Test substance	
Result	Sprague-Dawley rats were provided with 18, 25 and 32% protein-derived calories and 36% ethanol-derived calories in a liquid diet on gestation days 1-21. The maternal ethanol blood levels were 1.5-2 gll. Ethanol caused a significant decrease in fetal body weight and brain weight but an increase in relative brain weight. irrespective of the protein content of the diet.
Reliability	(4) not assignable
Reference	Weinberg. J. Effects of ethanol and maternal nutrition status of fetal development. Alcohol Clin Exp Res 1985;9 : 49-55.
12.11.2004	(340)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	
Strain	Sprague-Dawley
Route of admin.	oral unspecified
Exposure period	GD 16 until postnatal day 14 or from birth until postnatal day 14
Frequency of treatm.	
Duration of test	
Doses	36% of total calories in a liquid diet
Test substance	ethanol (64-17-5)
Result	The sexually dimorphic nucleus in the preoptic area of the brain of adult male offspring was significantly decreased in volume.
Reliability	(4) not assignable
Reference	Rudeen P.K.et a1.1986. Drug Alcohol Depend. 18, 247.
12.11.2004	(341)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	
Strain	Sprague-Dawley
Route of admin.	oral unspecified
Exposure period	GD 7-15
Frequency of treatm.	twice daily
Duration of test	3 day period
Doses	4g/kg
Test substance	ethanol (64-17-5)
Result	An increased incidence of resorptions and marginal effect on fetal body weight but no teratogenic effect were observed.
Reliability	(4) not assignable

Reference	Fernandez K. et al. 1983. Teratogen. Carcinogen. Mutagen. 3, 457.
12.11.2004	(342)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	Sprague-Dawley
Route of admin.	oral unspecified
Exposure period	
Frequency of treatm.	
Duration of test	Daily GD 1-15 or GO 1-20
Doses	5 or 5g/kg bodyweight
Test substance	ethanol (64-17-5)
Result	In contrast to studies in which gross malformations were not observed, polydactyly and polysyndactyly were reported in the offspring of rats given 5 g/kg bw (but not in those given 6 g/kg bw) per day ethanol. Maximal blood ethanol concentrations of 2.5-3.25 g/l were reported with the two doses.
Reliability	(4) not assignable
Reference	West J.R. et al. 1981a. Teratology 24, 13.
12.11.2004	(343)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	Long-Evans
Route of admin.	oral unspecified
Doses	Prenatal treatment with 35% ethanol-derived calories in a liquid diet.
Test substance	ethanol (64-17-5)
Result	Treatment shortened the umbilical cord.
Reliability	(4) not assignable
Reference	Barron S. et al. 1986. Alcohol. Clin. Exp. Res. 10, 493.
12.11.2004	(344)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	Long-Evans

Route of admin.	oral unspecified
Exposure period	GD 6-20
Frequency of treatm.	
Duration of test	
Doses	liquid diet containing ethanol as 35% of total calories
Test substance	ethanol (64-17-5)
Result	The most frequently reported behavioural teratogenic effect is alteration in motor activity. Increased motor activity of offspring was reported.
Reliability	(4) not assignable
Reference	Zimmerberg B. et al. 1986. Pharmacol. Biochem. Behav. 25, 1021.
12.11.2004	(345)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Mouse
Sex	Female
Strain	C3H
Route of admin.	oral unspecified
Exposure period	
Frequency of treatm.	
Duration of test	
Doses	1 x 1 ml of 12.5% alcohol; Estimate 2500 mg/kg.
Control group	
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Remark	The authors proposed that the effect was due to a specific action on the fertilized ovum at the time of second meiotic division, causing aneuploidy, but the numbers of embryos available for examination in this study were inadequate to confirm this hypothesis.
Result	Treatment of (C3H x C57BI)F1 female mice with a single dose of 1 ml of 12.5% ethanol by gavage 2 h after a 30-min mating period produced an increase in late (after day 11) fetal deaths. The same treatment given 1 hr after mating did not produce this effect.
Reliability	(4) not assignable
Reference	Washington, W.J.; Cain, K.T., Cacheiro, N.l.A., Generoso, W.M. Ethanol-induced late fetal death in mice exposed around the time of fertilization. Mutation Res 1985; 147: 205-210.

12.11.2004 (346)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Mouse
Sex	Male
Strain	C3H
Route of admin.	oral unspecified
Exposure period	4 weeks before mating
Frequency of treatm.	Daily
Duration of test	
Doses	20-30% of total calorie intake
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Male-mediated developmental effects Male C3H mice were fed ethanol (20 or 30% of total calories) in a liquid diet and, after four weeks of treatment, were mated to untreated females.
Result	The resulting litters showed no change in the number of implants, prenatal mortality, fetal weight, sex ratio or soft-tissue malformations.
Reliability	(4) not assignable
Reference	Randall, C.L., Burling, T.A., Lochry, E.A., Sutker, P.B. The effect of paternal alcohol consumption on foetal development in mice. Drug Alcohol Res 1982; 9: 89-95.

12.11.2004 (347)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Monkey
Sex	
Strain	other: Cynomolgus
Route of admin.	oral unspecified
Exposure period	GD 20-150
Frequency of treatm.	Daily
Duration of test	
Doses	5g/kg bw
Test substance	ethanol (64-17-5)
Result	An increase in pregnancy wastage (abortions and still births) was observed but no structural malformation or facial change.
Reliability	(4) not assignable
Reference	Scott W.J. & Fradkin R. 1984. Terotology 29, 46.

12.11.2004 (348)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	other: ferret
Sex	
Strain	
Route of admin.	oral unspecified
Exposure period	GD 15-35
Frequency of treatm.	
Duration of test	90 days prior to mating and during gestation or during gestation only
Doses	1.5g/kg bodyweight as a 25% solution
Test substance	ethanol (64-17-5)
Result	There was a significant increase in the number of fetuses and litters with malformations but no effect on fetal weight or resorptions. The peak blood ethanol concentration was 2 g/l.
Reliability	(4) not assignable
Reference	Mclain C.J. & Roe, 1984 (no further details available).

12.11.2004 (349)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	Long-Evans
Route of admin.	other: intragastric
Exposure period	GD 7-15
Test substance	ethanol (64-17-5)
Method	Administration of ethanol in combination with an unspecified extract of marijuana containing 9-tetrahydrocanabinol.
Result	Treatment produced a significant decrease in maternal weight gain and an increased incidence of resorptions. The incidence of resorptions was increased with marijuana alone, but the increase was more than additive with the combination of marijuana and ethanol.
Reliability	(4) not assignable
Reference	Abel E.L 1985 Teratology 31, 35.

12.11.2004 (350)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Mouse
Sex	
Strain	Swiss Webster

Route of admin.	s.c.
Exposure period	GD 1-15
Test substance	ethanol (64-17-5)
Method	Administration of ethanol in combination with an unspecified extract of marijuana containing 9-tetrahydrocanabinol.
Result	Treatment produced a significant decrease in maternal weight gain and an increased incidence of. resorptions. The incidence of resorptions was increased with marijuana alone, but the increase was more than additive with the combination of marijuana and ethanol.
Reliability	(4) not assignable
Reference	Abel E.L 1985 Teratology 31, 35.
12.11.2004	(350)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	other: hooded
Test substance	ethanol (64-17-5)
Method	
Result	In hooded rats given a liquid diet containing 37% ethanol-derived calories from day 6 of gestation to time of birth (gestation day 23 for ethanol exposed rats; day 22 for controls), delayed and extended period of cortical neuron generation, reduced number of neurons and altered distribution of neurons were seen.
Reliability	(4) not assignable
Reference	Miller NW. 1986. Science 233,1308.
12.11.2004	(351)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	other: albino
Test substance	ethanol (64-17-5)
Result	Ethanol in combination with lithium carbonate had a synergistic effect on the induction of fetal abnormalities.
Reliability	(4) not assignable
Reference	Sharma A. & Rawat A.K. 1986. Alcohol 3, 101.
12.11.2004	(352)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	Female
Strain	Long-Evans
Route of admin.	
Exposure period	60 days
Frequency of treatm.	
Duration of test	
Doses	20 ml of 20% alcohol; estimated 4000 mg/kg/day
Control group	
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	An increase in congenital malformations was noted.
Reliability	(4) not assignable
Reference	Mankes, R.F., LeFevre, R., Banitz, K.-F., et al. Paternal effects of ethanol in the LongEvans rat. J Toxicol Environ Health 1982; 10: 871-878.
12.11.2004	(353)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Rat
Sex	male/female
Strain	
Route of admin.	
Exposure period	40-45 days before mating and 5 days post fertilization
Frequency of treatm.	
Duration of test	
Doses	20% or 24% ethanol crudely calculated to 1100 mg/kg/day.
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Method	Preimplantation effects were studied by the examination of uterine contents of albino rats following consumption of plum brandy (reported as 24% ethanol) or cognac (reported as 20% ethanol) for 40-45 days before mating and during pregnancy until the rats were killed on day 5.
Result	Development was retarded, and there was an increased number of pathological morulae and blastocysts.

Reliability	(4) not assignable
Reference	Fazakas-Todea, I., Gheciu, Sandor, S. The effect of ethanol upon early development in mice and rats. VIII. The effect of chronic consumption of some beverages upon preimplantation development in rats. Morphol Embryol. 1985: 31: 249-256.
12.11.2004	(354)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	Female
Strain	Long-Evans
Route of admin.	
Exposure period	Days 6-15 of gestation
Frequency of treatm.	
Duration of test	
Doses	4000 mg/kg
Test substance	ethanol (64-17-5)
Result	In Long-Evans rats given 4 ml/kg bw ethanol as a single oral dose between days 6 and 15 of gestation, a variety of gross malformations was reported in 72-100% offspring compared to 12% of controls.
Reliability	(4) not assignable
Reference	Mankes, R.F., Hoffman, T., LeFevre, R.Bates, H., Abraham,R. Acute embryopathic effects of ethanolfn the long-Evans rat. J Toxicol Environ Health 1983; 11: 583-590.
12.11.2004	(355)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	Sprague-Dawley
Doses	15 or 25% ethanol-derived calories
Test substance	ethanol (64-17-5)
Method	Animals were given 15 or 25% ethanol-derived calories in liquid diets 20 days before mating, throughout mating and until gestation day 19; additional groups were pair-fed an isocaloric diet.
Remark	The effects of 15% ethanol-derived calories were attributed to ethanol, while the effects of 25% ethanol-derived calories were attributed partly to decreased caloric intake.
Result	There was decreased caloric intake in the group given 25% ethanol derived calories and in the pair-fed controls, and in both of these groups there were associated decreases in fetal body

	weight organ weights and DNA and protein contents compared to the pair-fed controls of the group given 15% ethanol-derived calories.
Reliability	(4) not assignable
Reference	Sorette M.P. et al. 1980. Neurobehav. Toxicol. 2, 181.
12.11.2004	(356)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Sex	
Strain	Long-Evans
Route of admin.	
Exposure period	throughout gestation
Frequency of treatm.	Daily
Duration of test	
Doses	4 or 6g/kg bw
Test substance	ethanol (64-17-5)
Remark	The most frequently reported behavioural teratogenic effect is alteration in motor activity.
Result	There was decreased litter weight but not litter size at birth and increased postnatal mortality. Motor activity of neonates raised by surrogate mothers was impaired at 16 and 20 days of age.
Reliability	(4) not assignable
Reference	Abel E.L. & Dintcheff BA 1978. J. Pharmacal. Exp. Ther. 207, 916.
12.11.2004	(357)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Rat
Test substance	ethanol (64-17-5)
Result	Behavioural teratogenic effects reported.
Reliability	(4) not assignable
Reference	Viirre E. et al. 1986. Neurobehav. Toxicol. Teratol. 8, 615. Vorhees C.V.& Fernandez K. 1986. Neurobehav. Toxicol. Teratol. 8, 23.
12.11.2004	(358) (359)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Mouse
Sex	
Strain	other: CF-1, CD-1, C3H

Test substance	ethanol (64-17-5)
Remark	Some studies in several mouse strains have shown no teratogenic effect even at dose levels providing blood ethanol concentrations of 2 g/l or higher. Mice given ethanol orally or in the drinking fluid had pups with minor skeletal variants or decreased fetal body weight, but there was no increase in resorptions or malformations.
Reliability	(4) not assignable
Reference	Hood R.D. et al. 1979. Toxicol. Lett. 4, 79. Lochry E.A. et al. 1982. Neurobehav. Toxicol. Teratol. 4, 15. Schwetz, B.A., Smith, FA, Staples, R.E. Teratogenic potential of ethanol in mice, rats and rabbits. Teratology 1978; 18: 385-392.
12.11.2004	(360) (361) (311)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Mouse
Test substance	ethanol (64-17-5)
Remark	Studies in mice showed teratogenic effects and resorptions. typically at blood ethanol concentrations in excess of 2 g/l. The effects, such as fetal resorptions, intrauterine growth retardation, cleft palate, altered craniofacial development and exencephaly, limb defects and heart defects, varied with the strain of mice, mode of administration and stage of gestation at which ethanol was administered.
Result	
Reliability	(4) not assignable
Reference	Bannigan J. & Burke P. 1982. Teratology 26, 247. Boggan W.O. et al. 1979. Res. Commun. Chem. Pathol. Pharmacal. 23, 127. Checiu M. & Sandor S. 1982. Morphol Embryol. 28, 15. Chernoff G.F. 1980. T eratology 22, 71. Chernoff, G. (1977). The fetal alcohol syndrome in mice: an animal model. Teratol. 15: 223-230. Daft P.A. et al. 1986. Teratology 33, 93. Giknis M.L.A. et al. 1980. Neurobehav. Toxicol. 7, 235.

Kronik J.B.1976. Am. J. Obstet. Gynecol. 124, 676.

Martinez F. et al.1985. Am. J. Obstet. Gynecol. 151, 428.
Padmanabhan R. & Muawad W.M.R.A. 1985. Drug Alcohol Depend. 16, 215.

Padmanabhan R. et al. 1984. Drug Alcohol Depend. 14, 197.

Randall C.L. et al. 1977. Alcohol Clin. Exp. Res. 1, 219.

Rasmussen B.B. & Christensen N. 1980. Acta pathol. Microbiol. Scand., Sect. A. 88, 285.

Stuckey E. & Berry C.L. 1984. J. Pathol. 142, 175.

Sulik KK et al. 1981. Science 214, 936.

Sulik KK & Johnston M.C. 1983. Am. J. Anal. 166, 257.

Webster W.S. etal.1980. Neurobehav. Toxicol. 2, 227.

Webster W.S. et al. 1984. Cardiovasc. Res. 18, 335.
12.11.2004 (362)(363)(364)(365)(307)(366)(367)(368)(369)(370)(371)(372)(373)(374) (375) (376) (377) (378)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Mouse
Sex	
Strain	Swiss Webster
Test substance	ethanol (64-17-5)
Result	Combined administration of ethanol and metronidazole increased the number of resporptions, decreased fetal body weight and had a marginal effect on the incidence of malformations.
Reliability	(4) not assignable
Reference	Giknis M.L.A. & Damjanov I. 1983. Toxicol. Lett. 19, 37.
12.11.2004	(379)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Species	Mouse
Sex	
Strain	Swiss Webster
Result	Ethanol increased the incidence of cleft palate in mice administered methyl mercuric chloride and retinyl acetate.

Reliability	(4) not assignable
Reference	Lee M. 1985. Teratogen. Carcinogen. Mutagen. 5, 433.
02.07.2004	(380)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Mouse
Test substance	ethanol (64-17-5)
GLP	
Remark	Behavioural teratogenic effects reported.
Reliability	(4) not assignable
Reference	Randall C.L. et al 1986. Alcohol Drug. Res. 6, 351. Yanai J. & Ginsburg B.E. 1976. Q. J. Stud. Alcohol 37, 1564.
12.11.2004	(381) (382)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Miniature swine
Sex	Female
Strain	
Route of admin.	
Exposure period	Throughout gestation
Frequency of treatm.	
Duration of test	Throughout gestation
Doses	3000 and 3600 mg/kg/day
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	In miniature swine given 20% ethanol in drinking-water (>3 g/kg bw/day) as gilts (18 months old) or sows (three years old), there was a significant decrease in mean litter size and in the birth weight of piglets and a significant increase in the incidence of multiple malformations.. There was a slight decrease in the number of offspring per litter; there was also a slight decrease in still births. Open-field activity was significantly increased in offspring.
Reliability	(4) not assignable
Reference	Dexter, J.D., Tumbleson, M.E., Decker, J.D., Middleton, C.C. Fetal alcohol syndrome in Sinclair (S-1) miniature swine. Alcohol Clin Exp Res 1980; 4: 146-151.
12.11.2004	(383)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Species	Monkey
Sex	Female
Strain	
Route of admin.	
Exposure period	Days 20-150 of gestation
Frequency of treatm.	
Duration of test	
Doses	5000 mg/kg/day
Control group	no data specified
Method	other
Year	
GLP	no data
Test substance	95 – 99.9% ethanol (64-17-5)
Result	There was an increase in abortions and stillbirths but no structural or skeletal (facial) deformities.
Reliability	(4) not assignable
Reference	Scott, W.J. Jr., Fradkin, R. The effects of prenatal ethanol in Cynomolgus monkeys. Teratology 1984; 29:49-56.
12.11.2004	(384)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Remark	Ethanol at high blood levels has caused significant reductions in foetal body weight, increased resorptions and teratogenic effects in a number of species. Some, though not all, studies in mice and rats have demonstrated altered behavioural development following exposure to ethanol in utero. Exposure in utero or during lactation reduced postnatal growth.
Reliability	(4) not assignable
Reference	IARC Monographs. (1988) Volume 44. Alcohol Drinking. Lyon, France.
06.07.2004	(18)

<u>Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)</u>

Remark	When 20% ethanol in water (v/v) was given as the drinking fluid for 60 days to male Long-Evans rats, which were mated with untreated females one to three weeks after cessation of treatment, the incidence of congenital malformations in the offspring was increased
Reliability	(4) not assignable
Reference	Mankes R.F. et al. 1982. J. Toxicol. Envir. Hlth 10, 871.
12.11.2004	(385)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Remark	In a study to evaluate the role of zinc deficiency in the developmental toxicity of ethanol, CBA/J mice were given a liquid diet, either fortified with zinc or deficient in zinc, and ethanol (15 or 20% of total calories).
Result	Zinc deficiency potentiated the ethanol-induced increase in resorptions and external malformations and the decrease in fetal weight.
Reliability	(4) not assignable
Reference	Keppen L.D. et at 1985. Pediat. Res. 19, 944.
12.11.2004	(386)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Remark	Among offspring of Long-Evans rats fed liquid diets containing 35% ethanol-derived calories during gestation days 6-20, there was evidence of behavioural deficits, which persisted until adulthood. Female offspring showed a variety of deficits in maternal behaviour when adult, which may have been related to prenatal hormonal alterations
Reliability	(4) not assignable
Reference	Barron S. & Riley E.P. 1985. Alcohol. Clin. Exp. Res. 9, 360.
12.11.2004	(387)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Remark	There was an increase in the incidence of both external and internal malformations in C57BI/6 mice given a marginally zinc deficient diet and ethanol during gestation, in comparison with mice given a control diet and with mice treated with ethanol alone.
Reliability	(4) not assignable
Reference	Miller S.I. et al. 1983. Pharmacol. Biochem. Behav. 18, 311.
12.11.2004	(388)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Remark	When ethanol is given in combination with other chemicals which tend to increase the blood level of ethanol by reducing its metabolism, e.g. 4-methylpyrazole and pyrazole, the teratogenic and fetotoxic effects are increased.
Reliability	(4) not assignable
Reference	Blakley P.M.& Scott W.J. 1984b. Toxic. Appl. Pharmac. 72, 355. Varma PK & Persaud T.V.N.1979. Res. Commun. chem. Palthol. Pharmacol. 26, 65.

12.11.2004 (389) (390)

Ethanol (64-17-5) for Ethanol Aluminum Salt (555-75-9)

Remark	Administration of ethanol with chemicals that tend to increase the acetaldehyde level, e.g. disulfiram does not increase the teratogenicity of ethanol.
Reliability	(4) not assignable
Reference	Webster W.S. et al.1983. Teratology 27, 231.
12.11.2004	(391)

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Species:	rat
Strain:	Sprague-Dawley
Sex:	male and female
Route of Admin.	inhalation
Exposure Period:	Day 1-20 of gestation
Freq. of Treatment:	7 hours/day
Duration of Test:	20 Days
Exposure Concentrations:	0, 3000, or 6000 ppm of n-butanol
Control Group:	Yes
NOAEL Maternal Toxicity:	not reported
NOAEL Developmental Neurotoxicity:	6000 ppm
Method:	Groups of 18 male Spragne-Dawley rats were exposed to concentrations of 0, 3000, or 6000 ppm nBA for 7 hours/day for 6 weeks. These males were then mated to non-exposed female rats of the same. strain. In a separate experiment, groups of 15 pregnant female rats were exposed to concentrations of 0, 3000, or 6000 ppm for 7 hours/day from gestation Day 1-20. These females were then allowed to deliver. The offspring from these two groups were. then observed for signs of developmental neurotoxic effects. Offspring were examined from postnatal days 10-90 for the following measures: ascent on a wire mesh screen, rotorod, open-field and photoelectrically-monitored activity, running wheel, avoidance conditioning, operant conditioning, acetylcholine, dopamine, norepinephrine, serotonin, met-enkephalin, beta-endorphin, and Substance P. neurotransmitter levels were measured from the cerebrum, cerebellum, brainstem, and midbrain.
Year:	1989
GLP:	No
Test substance:	n-Butanol purity> 99%
Result:	No detectable effect on pregnancy rate was found after either

maternal or paternal exposure. In the 6000 ppm group, 4 of the 78 (5%) behavioural measures, and 4 of the 64 (6%) neurochemical measures differed from those of controls. There was no discernible pattern of effects. The authors conclude, "In view of this, it is highly unlikely that administration of nBA at the current Permissible Exposure Limit (PEL) of 100 ppm would produce structural or behavioural teratogenicity in rats using the test employed here.

Reference: Nelson, B.K., Brightwell, W.S., Robertson, S.K., Kahn, A., Krieg, E.F., lr. and Massari, V.l. Behavioral Teratology investigation of 1-Butanol in Rats. Neurotoxicology and Teratology. 11(3): 313-315, 1989a.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Species: rat
Strain: Sprague-Dawley
Sex: female
Route of Admin. inhalation
Exposure Period: Day 1-19 of gestation
Freq. of Treatment: 7 hours/day
Duration of Test: 20 Days
Exposure Concentrations: 0, 3500, 6000 or 8000 ppm of n-butanol
Control Group: Yes
NOAEL Maternal Toxicity: 3500 ppm
NOAEL Developmental Neurotoxicity: 3500 ppm
Method: Groups of approximately 15 pregnant Sprague-Dawley rats were exposed via inhalation to 0, 3500, 6000 or 8000 ppm of n-butanol for 7 hours/ day from gestation Day 1 - 19. On gestation day 20, the fetuses were collected and examined for both skeletal and visceral malformations.
Year: 1989

GLP: No
Test substance: n-Butanol purity> 99%
Result: 8000 ppm produced narcosis in approximately one-half of the dams. No behavioural effects were noted at 6000 ppm nBA. Two of eighteen dams at 8000 ppm died during the exposure period. Feed censumptien was decreased in the 6000 and 8000 ppm nBA exposed dams, but the 3500 ppm dams were similar to controls. No effect was observed on mean corpora lutea/litter, mean resorptions/litter, mean number of live foetuses/litter or sex ratio. Foetal weights were slightly decreased at 6000 and 8000 ppm groups, but the 3500 ppm group was unaffected.

External foetal malformations were not observed. There were no differences in malformation rates (skeletal or visceral) or in rates of commonly observed variations. However, there was a slight increase in the percent of fetuses with any skeletal variation or malformation in the 8000 ppm group but not in the lower two expesure groups. The authors concluded that although high concentrations (8000 ppm) of nBA produced developmental texicity, it was not a strong developmental toxicant. The NOAEL for maternal animals was 3500 ppm and the NOAEL fer offspring was 3500 ppm (based on slight decrease in foetal weight at 6000 ppm).

Reference: Nelson, BK., Brightwell, WS., Kahn, A., Burg, JR. and Goad, PT. Lack of selective developmental toxicity of three butanol isomers administered by inhalation to rats. Fundamental and Applied Toxicology. 12(3):469-479.,1989b.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Species: n-butanol
Strain: Rat, Imp:DAK; internal breeding colony to the Nufer Institute of Occupational Medicine in Lodz, Poland
Sex:
Number of Animals 11-17/group
Route of Admin. Aqueous solutions for drinking water
Exposure Period: 8 weeks premating, 3 weeks mating, gestation Days 0-20
Freq. of Treatment: Daily
Post Exposure: None
Duration of Test: Premating (8 weeks), mating (up to 3 weeks), gestation (20 days)

Exposure Concentrations: 0.24, 0.8, or 4% n-butanol (0.3, 1.0, and 5.0 grams/kg/day)
Control Group: Yes, vehicle control
NOAEL: Not reported (questionable)
LOAEL: 0.3 grams/kg/day (highly questionable)
Method: Groups of 11-17 female rats were given aqueous solutions containing 0.24, 0.8, or 4% n-butanol for 8 weeks prior to mating, during which time estrous cyclicity was evaluated. After the 8 week exposure period (with no effects on estrous cyclicity), the females were mated with untreated males. The females had continued access to the solutions of n-butanol (above) in the water until Day 20 of gestation when they were killed and the fetuses were collected and examined for both skeletal and visceral malformations. Weight gains and feed consumption as well as general behavior were recorded during the 8 week premating period, 3 week mating period and gestation. The authors state that the aqueous solutions delivered 0.3, 1.0, and 5.0 grams/kg/day, although there is no information

as to how this was determined. The 4% solution was described as delivering daily doses twice as high as the acute. oral LD50 (2.1 grams/kg/day). The unit of statistical analysis was the individual fetus, not the litter.

Test Result: General appearance, feed consumption, body weights, rate of weight gain, estrous cycle length and number, absolute and relative organ weights (not specified), hemoglobin concentrations, hematocrit values, fetal body weights, intrauterine mortality, corpora lutea, total implants, and placental weights were unaffected. At 4% n-butanol in the drinking water, the crown-rump length is decreased from a control mean of 4.0 cm to 3.8 em. The authors report developmental anomalies in all three dose levels. Fetal skeletal effects were limited to extra 14th rib (1 fetus in the low dose group and 2 fetuses in the high dose group), and wavy ribs (1 fetus in the low dose group). Central nervous system defects were limited to dilation of either the subarachnoid space or lateral and/or third ventricles of the brain, dilated renal pelvis, or external or internal hydrocephalus. Of the 65 control fetuses examined for skeletal effects, none had an extra 14th rib or wavy ribs(s) or any other skeletal malformation or variation. Of the 61 control fetuses examined for visceral observations, 2 had dilatation of the lateral and/or third ventricles of the brain and none had dilatation of the subarachnoid space or internal or external hydrocephalus. Although the authors considered all three dose levels to have increased levels of defects when compared to controls, there was no increase in incidence from the low exposure concentration (0.24% n-butanol; 0.3 grams/kg/day) to the high exposure concentration (4% nbutanol; 5.0 grams/kg/day).

GLP: No

Comments: Developmental anomalies reported by the authors (dilatation of the brain ventricles/spaces or renal pelvis, internal hydrocephalus, wavy or extra ribs) as being due to n-butanol exposure are listed as variations or delayed development in commonly used historical databases. Of importance, the incidence of these developmental defects in the control population was zero percent (with the exception of 2/61 pups with brain dilatation). The incidence of "cerebral ventricle, enlargement" was 2% on a per fetus basis and 4.4% on a per li tter basis in the 199 5 MART A/MT A reference database for Sprague-Dawley rats (this is a database of common malformations/variations in control animals in studies conducted in the USA). The incidence of "renal pelvis, dilated" was 0.95% on a per fetus basis and 5.2% on a per litter basis in

the same reference database. However, the "malformations reported in this paper that are termed "variations" in other established databases have to be classified based upon the incidence within the specific rat strain. The incidence of variations within the Tat strain used in this study is unknown since the authors used a rat strain common only to their laboratory in Poland. The laboratory feed was also unique to their laboratory in Poland. Since the strain of rat and type and quality of diet can have a profound effect on rates or variations and malformations and since there is no historical database for these animals, the term "variation" has to be assigned with reservation. However, since these variations are common to several rat strains commonly used in the United States, the term "variation" appears appropriate. In fact, the data from Nelson, et al, (1989a) also reports some of these variations following inhalation exposure. It should not be surprising that high oral doses of n-butanol that would be expected to alter normal maternal physiology would cause an increase in common variations in laboratory rodents.

Reference: Sitarek, K., Berlinska, B., and Baranski, B. Assessment of the Effect of n-Butanol Given to Female Rats in Drinking Water on Fertility and Prenatal Development of Their Offspring. Int. J. of Occupational Medicine and Environmental Health, 7(4): 365-370, 1994.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Preferred Value: Score= 1
Species: rat
Strain: Sprague-Dawley
Sex: female
Route of Admin. inhalation
Exposure Period: Group 1-Control
Group 2- Day 7-16 of gestation
Group 3- Day 1-16 of gestation
Group 4- 3 weeks prior to mating and from Day 1-16 of gestation
Freq. of Treatment:
Premating, 7h/day, 5 day/week
During gestation, 7h/day, 7 days/week

Duration of Test: Variable (see exposure period)
Exposure Concentrations: 1,500 ppm (7,230 mg/mg3)
Control Group: yes, concurrent no treatment
LOAEL Maternal Toxicity: 1,500 ppm

NOAEL Teratogenicity: 1,500 ppm

Method: Four groups, each containing 37-43 female Sprague-Dawley rats were. exposed to n-butyl acetate air concentrations of either o or 1,500 ppm for 7 hours/day. The rats were maintained in the exposure chambers throughout the study period, 3 weeks pregestation until gestation day 21. Group 1 was not exposed to test material throughout the study and served as the control. Group 2 was exposed to 1,500 ppm n-butyl acetate from day 7 to 16 of gestation. Group 3 received n-butyl acetate from Day 1 to 16 of gestation and Group 4 was exposed from 3 weeks pregestation through day 16 of gestation. All test material exposures were discontinued from gestation day 17 through study termination. Premating exposures were for 5 days/week while gestational exposures were continuous. On gestation Day 21 (sperm positive Day 1), the fetuses were collected and examined for both skeletal and visceral malformations. Vapor atmospheres of n-butyl acetate were generated using a heated, stainless steel vaporizer with vapor concentrations controlled by a pump metering the amount of liquid available. The chambers were 2.3 m3 in volume and exposure concentrations were. within 3% of target.

Year: 1982

GLP: yes

Test substance: n-butyl acetate, purity 99%

Result: Feed consumption was decreased in each test group in the week following initiation on n-butyl acetate exposure. The decrease in feed consumption was accompanied by decreases in body weight in Groups 1 and 4. Relative kidney and lung weights were. increased in animals exposed to n-butyl acetate, with the greatest increase occurring in the animals receiving the longest exposure. There were no changes in histopathology that could be related to n-butyl acetate exposure. Mating and reproductive performance and intrauterine mortality was unaffected. Fetal growth measures (fetal body weights and crown-rump growth) and placental weights were lower in Groups 2, 3, and 4. However, the duration of exposure and period of gestation during which exposure occurred did not affect fetal growth indices. Sex ratios were unaffected. There was no increase in the incidence of "Major Malformations" in any of the n-butyl acetate exposed groups. There was an increase in the incidence of the skeletal anomalies ("total rib dysmorphology") and in skeletal variation "reduced ossification of the pelvis" in Groups 2 and 3, but not in Group 4. The incidence of rib dysmorphology in the control population was zero. Group 4 had an increased incidence in "hydroureter" when compared to the control group (Group 1). Groups 2 and 3 were unaffected. The

lack of a uniform response between Groups 2,3, and 4 for the effects noted above that should have occurred during the same exposure period (Gestation Day 7-16), led the authors to conclude, "We hesitate to define this as a teratogenic effect of n-butyl acetate, since a similar increase was not seen in the group of rats exposed during this period of gestation subsequent to a pregestational exposure."

Reference: Hackett, P.L., M.G. Brown, R.L. Buschbom, M.L. Clark, R.A. Miller, R.L. Music, S.E. Rowe, R.E. Schirmer, and M.R. Sikov. 1982. Teratogenic Study of Ethylene and Propylene Oxide and n-Butyl Acetate. Prepared by the U.S. Department of Health and Human Services. Public Health Service. Center for Disease Control. National Institute for Occupational Safety and Health. Division of Biomedical and Behavioral Science. Experimental Toxicology Branch, Cincinnati, Ohio 45266. NTIS PB83258038.

1-Butanol (71-36-3) for 1-Butanol Aluminum Salt (3085-30-1)

Preferred Value: Score = 1
Species: Rabbit
Strain: New Zealand White
Sex: female
Route of Admin. inhalation
Exposure Period: Group 1- Control
Group 2- Day 7-19 of gestation
Group 3- Day 1-19 of gestation

Freq. of Treatment: 7 hours/day

Duration of Test: variable
Exposure Concentrations: 1,500 ppm (7,230 mg/m3)
Control Group: yes, concurrent no treatment
LOAEL Maternal Toxicity: 1,500 ppm
NOAEL Teratogenicity: 1,500 ppm
Method: Three groups of 21-25 female New Zealand White rabbits were exposed to n-butyl acetate air concentrations of either 0 or 1,500 ppm. Rabbits in all groups were placed in exposure chambers for 7-hours per day from study day 1 to 19. The rabbits were housed outside of the exposure chambers between exposure (sham or test material) periods. Group 1 received sham exposures to filtered air throughout the study and served as controls. Group 2 was exposed to 1,500 ppm n-butyl acetate from Day 7 to 19 of gestation. Group 3 was exposed to test

material from gestation Day 1 to 19. All test material exposures were discontinued from gestation Day 20 through study termination. On gestation Day 30 the fetuses were collected and examined for both skeletal and visceral malformations. Feed consumption and body weight data were recorded. Vapor atmospheres ofn-butyl acetate were generated using a heated, stainless steel vaporizer with vapor concentrations controlled by a pump metering the amount of liquid available. The chambers were 2.3 m3 in volume and exposure concentrations were within 3% of target.

Year: 1982

GLP: yes

Test substance: n-butyl acetate, purity 99%

Result: Feed consumption was. decreased in Groups 2 and 3 in the week following initiation of n-butyl acetate exposure. However, feed consumption was always lowest in Group 1 (controls). The body weight in Groups 2 and 3 were consistently higher than Group 1. Organ weights and histopathology were unremarkable in the n-butyl acetate exposed animals. Mating and reproductive performance and intrauterine mortality was unaffected for nbutyl acetate exposure. Fetal growth measures (fetal body weights and crown-rump length), placental weights, and sex ratios were not affected by n-butyl acetate exposures. There was no increase in the incidence of "Major Malformations" in any of the n-butyl acetate exposure groups. In terms of "Minor Anomalities," there was an increase in the incidence of "misaligned sternabra" and "retinal folds" in Group 3; Group 2 was not affected. Only a single increased incidence of "Morphologic Variations" was found, an increase in "clear gallbladder"; and that only in Group 3. The authors concluded that rabbit fetuses were unaffected by n-butyl acetate exposure based upon a lack of uniform response between the two exposure groups.

Reference: Hackett, P.L., M.G. Brown, R.L. Buschbom, M.L Clark, R.A. Miller, R.L. Music, S.B. Rowe, R.E. Schirmer, and M.R. Sikov. 1982. Teratogenic Study of Ethylene and Propylene Oxide and n-Butyl Acetate. Prepared by the U.S. Department of Health and Human Services. Public Health Service. Center for Disease Control. National Institute for Occupational Safety and Health. Department of Biomedical and Behavioral Science. Experimental Toxicology Branch. Cincinnati, Ohio 45266. NTIS PB83-258038.

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: rat **Sex:** female

Strain: Sprague-Dawley
Route of administration: inhalation
Exposure period: days 1-19 of gestation
Frequency of treatment: 7 hours/day
Duration of test: 20 days
Doses: 3500 mg/m3
Control Group: yes
NOAEL Maternal Toxity: = 3.5 mg/l
NOAEL Teratogenicity: = 3.5 mg/l

Method: other: see text
Year: 1989
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: NOAEL : 3.5 mg/l for maternal and foetal toxicity. No evidence of maternal toxicity, foetotxicity or teratogenicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: Within 5% of the nominal concentration of 3.5 mg/l when measured by Infrared analysis. This is the highest attainable dose under the conditions of the study.

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: Not reported
- Number aborting: Not reported
- Number of resorptions: There was a significant increase in mean resorption/litter ($p<0.05$). 1-hexanol treated 1.3, controls 0.4. This was within the historical control range which is reported as up to 1.3 resorptions per litter. The actual control value was at the lower end of the range of values found among 11 control groups used in a series of similar studies by these authors over a 5 year period (Nelson et al 1990b). The range of resorptions in these control groups was 0.2 -1.5 per litter (mean 0.9) further suggesting that this was not a treatment related effect.
- Number of implantations: Values not given although as numbers were recorded assume there was no difference between treated and controls.
- Number of corpora lutea: Comparable between treated and control groups. Corpora lutea/litter controls 17 +- 1, treated 14 +- 4.
- Duration of Pregnancy: Not reported.

- Body weight: Weight gain was comparable in treated and

control groups.
- Food/water consumption: Food consumption significantly higher than controls ($p<0.05$); water consumption unaffected.
- Description, severity, time of onset and duration of clinical signs: None
- Hematological findings incidence and severity: Not carried out.
- Clinical biochemistry findings incidence and severity: Not carried out.
- Gross pathology incidence and severity: Not carried out.
- Organ weight changes: Not carried out.
- Histopathology incidence and severity: Not carried out.

FETAL DATA:
- Litter size and weights: Comparable between treated & control groups. Mean foetal weight treated - males 3.19 g, females 3.05g; controls - males 3.28 g, females 3.19 g. Litter size (mean) treated and control 15.
- Sex ratio: No significant difference between treated and controls. Sex ratio - controls 7F, 8M; Treated 8F,7M.
- Grossly visible abnormalities: None
- External abnormalities: None
- Soft tissue abnormalities: None
- Skeletal abnormalities: There were small insignificant delays in ossification of caudal vertebrae, sternum, metacarpals and hind paw phalanges indicative of growth retardation but which were not accompanied by effects on foetal weight. Data not presented.

Source: Nelson, et al. 1989.
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS
Groups of approximately 15 female rats weighing 200-300g at the beginning of pregnancy.

ADMINISTRATION / EXPOSURE
- Type of exposure: Inhalation, concentrations monitored continuously and recorded hourly.
- Duration of test/exposure: 7 hours a day from day 1-19 of gestation.
- Dose: 3.5 mg/l which was the highest atmospheric concentration which could be generated at a temperature below 80F.

MATING PROCEDURES: Sperm positive females used, no other information.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily for 1st week then weekly
- Food & water consumption: Weekly on days 7, 14 and 20.
- Clinical observations: Assume daily frequency not actually reported.
- Examination of uterine content: Gestation day 20 ovaries also removed with uterus for examination of corpora lutea, implantations, resorption sites and live foetuses recorded.
- Examination of fetuses: Gestation day 20 examined for external, visceral and skeletal anomalies. Foetal weights and sex were recorded.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
Not carried out.

STATISTICAL METHODS: Multivariate analysis of variance (MANOVA) and ANOVA

Conclusion: The NOAEL for maternal toxicity, foetotoxicity and teratogencity in rats, following inhalation exposure to n-hexanol on gestation days 1-19, is 3.5 mg/l (850 ppm), the highest atmospheric concentration which could be generated. There was no maternal toxicity based on clinical observations and bodyweight measurement. Reproductive indices were unaffected by treatment. An apparent increase in the number of resorptions was within historical control limits and within the limits of a series of control groups from comparable studies. Combined with the particularly low incidence of resorptions in the control groups this observation is not considered treatment related.
Reported in Iuclid 2000 and Patty 2001.

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau hexan-1-ol Cas# 111-27-3

Nelson, B.K., Brightwell, W.S., Khan, A., Krieg, E.F., Jr., and Hoberman, A.M. 1989. Developmental toxicology evaluation of 1-pentanol, 1-hexanol, and 2-ethyl-1-hexanol administered by inhalation to rats. J. Am. Coll. Toxicol. 8(2): 405-410.

Nelson, B.K; Brightwell, W.S; Kreig, E.F. 1996 Developmental toxicology of industrial alcohols: A summary of 13 alcohols

administered by inhalation to rats. Tox. Ind. Hlth. 6(3/4): 373-387.

Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.
11-MAY-2006 (29) (43) (44) (48)

1-Hexanol (111-27-3) for 1-Hexanol Aluminum Salt (23275-26-5)

Species: rat **Sex:** female
Strain: other: COBS CD
Route of administration: gavage
Exposure period: days 6-15 of gestation
Frequency of treatment: daily
Duration of test: through day 20 of gestation
Doses: 200 and 1000 mg/kg bw
Control Group: yes
NOAEL Maternal Toxity: = 200 mg/kg bw
NOAEL Teratogenicity: = 1000 mg/kg bw

Method: other: see text
Year: 1988
GLP: no data
Test substance: >95% 1-hexanol (111-27-3)

Result: Maternal toxicity at 1000 mg/kg/day was evidenced by reduced body weight and clinical signs of intoxication. No further details are available. There were no signs of maternal toxicity at 200 mg/kg/day.

There was no evidence of teratogenicity in this study. Effects on the foetus were confined to an increase in numbers of litters with the skeletal variant 'malaligned sternebrae'

which occured at 200 mg/kg/day only and a slight decrease in foetal weight at 1000 mg/kg/day which was within the historical control range.

As an increased incidence of 'malaligned sternebrae' was not observed at 1000 mg/kg/day the observation at 200 mg/kg/day was considered incidental.
Source: Rodwell 1988.
Hayes Consultancy Service Bromley, Kent
Test condition: Summary data only are available for this study. Groups of 25 bred female COBS CD rats received either 200 or 1000 mg/kg/day 1-hexanol daily by gavage on gestation days 6-15. the test

material was administered in corn oil at a volume 5 ml/kg, a vehicle control group was included. Appearance, behaviour and body weights were recorded throughout the gestation. The dams were sacrificed and sectioned on gestation day 20. Intrauterine survival, foetal weight and external, skeletal and visceral anomalies were recorded.

Conclusion: The NOAEL for maternal toxicity in rats, following exposure by gavage to n-hexanol on gestation days 6-15, is considered to be 200 mg/kg/day based on clinical signs of toxicity and reduction in bodyweight at the higher dose level of 1000 mg/kg/day. The NOAEL for teratogenicity and foetotoxicity is considered to be 1000 mg/kg/day based on absence of adverse effects at this dose level (highest tested). A slight decrease in foetal weights was within historical control limits. Reported in Patty 2001.

Reliability: (4) not assignable
Abstract only available.

Reference: Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

Rodwell, D.E., Mercieca, M.D., Rusch, G.M., and Tasker, E.J. 1988. A teratology screening study in rats with n-hexanol. Toxicologist 8 (1): 213. (Abstract only).

11-NOV-2004 (48) (54)

<u>1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)</u>

Species: rat **Sex:** female
Strain: Wistar
Route of administration: gavage
Exposure period: gestation days 6-15
Frequency of treatment: daily
Duration of test: 20 days
Doses: 0, 130, 650, 975, and 1,300 mg/kg/day
Control Group: yes
NOAEL Maternal Toxity: = 130 mg/kg bw
NOAEL Teratogenicity: = 1300 mg/kg bw

Method: other: Closely followed EEC directives 87/302/EEC and 67/548/EEC and OECD Guideline No. 414
Year: 1997
GLP: yes
Test substance: > 90% 1-octanol (111-87-5)
Method: Divergence from test method by using 10 animals/group instead of 20.
Result: NOAEL: The NOAEL for maternal toxicity is 130 mg/kg/day based

on overt maternal toxicity at higher dose levels. There were no treatment related effects on the foetus and the NOAEL for teratogencity and foetotoxicity is 1300 mg/kg.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 130, 650, 975 and 1300 mg/kg/day (some problems with the detection method suggest that the actual dose administered at the top dose levels may have been larger than the nominal value)

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: Two dams died in the top dose group (1300 mg/kg/day) and a further 2 in the 650 mg/kg/day group.
- Number pregnant per dose level: water control 9, aqueous emulsifier 10, 130 mg/kg 10, 650 mg/kg 9, 975 mg/kg 8, 1300 mg/kg 8.
- Number aborting: None
- Number of resorptions: Comparable in treated and control groups. Resorptions (all)/dam (mean) 1.0, 1.4 (controls); 1.2, 0.7, 0.8 and 1.3 treated groups low - high.
- Number of implantations: Comparable in treated and control groups. Implantation site/dam (mean) 14.7, 16.0 (controls); 14.7, 15.4, 13.8 and 14.5 treated groups low - high.
- Post implantation loss: Comparable in treated and control groups.
- Number of corpora lutea: Comparable in treated and control groups. Corpora lutea/dam (mean)14.8, 16.3 (controls); 15.0, 16.0, 14.9 and 14.5 treated groups low - high.
- Duration of Pregnancy: Comparable in treated and control groups.
- Body weight: A slight decrease in body weight gain in the 650, 975 and 1300 mg/kg treated groups from day 15 to the end of the study was not of statistical significance.
- Food/water consumption: A slight decrease (magnitude not reported) in food consumption was reported in the 650, 975 and 1300 mg/kg treated groups.
- Description, severity, time of onset and duration of clinical signs: There was a dose related increase in signs of maternal toxicity observed at all dose levels with increasing severity. The effects at the lowest dose level 130 mg/kg/day were marginal. Signs observed were assumption of a lateral or abdominal position, piloerection, unsteady gait, salivation, nasal discharge and pneumonia.
- Hematological findings incidence and severity: not carried out
- Clinical biochemistry findings incidence and severity: Not

carried out.
- Gross pathology incidence and severity: Not reported
- Organ weight changes: Uterine weight and placental was unaffected by treatment.
- Histopathology incidence and severity: Not carried out.

FETAL DATA:
- Litter size and weights: Comparable in treated and control groups.
- Number viable: Viability was comparable to controls. Live foetuses/dam (mean) 13.7, 14.6 (controls); 13.5, 14.7, 13.0 and 13.2 treated groups low to high.
- Sex ratio: Not reported.
- Total malformations, variations and retardations: The incidence was unaffected by treatment. All foetal values were within the range of biological variation. Differences in malformations or retardations were not statistically significant and without dose relationship. A single cheiloschisis and one anophthalmy in the top dose group were considered incidental and not related to treatment. Litters with malformations number (%) 2 (22), 3 (30) (controls); 3 (30), 3 (43), 2 (25) and 1 (17) treated groups low to high. Litters with variations number (%) 8 (89), 10 (100) (controls); 10 (100), 7 (100); 7 (88) and 5 (83) treated groups low to high. Litters with retardations number (%) 8 (89), 9 (90) (controls); 9 (90), 7 (100), 8 (100) and 5 (83) treated groups low to high.

Source: Hellwig and Jackh 1997
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS
- Groups of 8-10 pregnant Wistar rats aged 68-85 days at study initiation, mean weight 214-233 g

ADMINISTRATION / EXPOSURE

- Type of exposure: gavage
- Duration of test/exposure: treatment day 6-15 post coital, termination day 20 post coital.
- Treatment: 130, 650, 975 and 1300 mg/kg/day
- Control group and treatment: two control groups were used one with twice distilled water and one with 0.005% Cremophor EL as emulsifier.
- Vehicle: 0.005% Cremophor in water
- Concentration in vehicle: Adjusted to give constant volume
- Total volume applied: 5 ml/kg

MATING PROCEDURES: 1 fertile male to 4 females.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily
- Food consumption: Daily
- Clinical observations: Daily
- Examination of uterine content: At gestation day 20, uterine weight, numbers of implantations shown as: live foetuses, dead implantations, early resorptions (stained), early & late resorptions (unnstained), dead foetuses. Conception rates and pre & post implantational losses were calculated.
- Examination of fetuses: Foetal weights, external, visceral and skeletal anomalies, variations & retardations, unclassified observations.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
Not reported

STATISTICAL METHODS: Dunnetts test for most reproductive parameters and Fischers exact test for evaluaton of conception rate and all foetal findings.

Conclusion: Administration of n-octanol to pregnant female rats by gavage on gestation days 6-15 caused dose related overt clinical signs of toxicity (irritation and transient CNS depression) at dose levels in excess of 130 mg/kg/day. However there were no treatment related effects on the offspring or reproductive parameters monitored and the NOAEL for teratogenicity and foetotoxicity is 1300 mg/kg/day with a maternal NOAEL of 130 mg/kg/day.

Reliability: (2) valid with restrictions
Comparable to guideline study with acceptable restrictions (Group sizes are smaller than recommended 8-10 pregnant females rather than 20).

Flag: Critical study for SIDS endpoint

Reference: Hellwig, J. and Jackh, R. 1997. Differential prenatal toxicity of one straight-chain and five branched-chain primary alcohols in rats. Food and Chem. Toxicol. 35: 489-500.

11-MAY-2006 (47)

<u>1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)</u>

Species: rat **Sex:** female
Strain: Sprague-Dawley
Route of administration: inhalation

Exposure period: 19 days
Frequency of treatment: 7 hours/day
Duration of test: 20 days
Doses: 400 mg/m3
Control Group: yes
NOAEL Maternal Toxity: > .4 mg/l
NOAEL Teratogenicity: > .4 mg/l

Method: other: see text
Year: 1990
GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Remark: The results reported in the primary reference (Nelson et al, 1990) are summarised in a comparative review of 13 alcohols tested by the same author (Nelson et al, 1996). The test concentration for n-octanol is apparently misquoted in Nelson 1990b as the original reference gives the test concentration as 400 mg/m3. The erroneous value (350 mg/m3) is carried through to Patty 2001.

Result: NOAEL : 0.4 mg/l for maternal and foetal toxicity. No evidence of maternal toxicity, foetotoxicity or teratogenicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: Within 5% of the nominal concentration of 0.4 mg/l when measured by Infrared analysis. This is the highest attainable dose under the conditions of the study. Actual dose achieved 0.402 mg/l.

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: Not reported
- Number aborting: Not reported
- Number of resorptions: Comparable in treated and control groups. Mean resorptions/litter control 0.5, treated 0.4.
- Number of corpora lutea: Comparable between treatd and control groups. Mean corpora lutea/litter control 14.0, treated 14.8.
- Duration of Pregnancy: Not reported.
- Body weight: Weight gain was comparable in treated and control groups.
- Food/water consumption: Comparable between treated and control groups.
- Description, severity, time of onset and duration of clinical signs: None
- Hematological findings incidence and severity: Not carried

out.
- Clinical biochemistry findings incidence and severity: Not carried out.
- Gross pathology incidence and severity: Not carried out.
- Organ weight changes: Not carried out.
- Histopathology incidence and severity: Not carried out.

FETAL DATA:
- Litter size and weights: Comparable between treated & control groups. Litter weights control males 3.22g, females 3.12g; treated males 3.56g, females 3.44g.
- Sex ratio: No significant difference between treated and controls. Control males/litter 6.6, females 6.9; treated males 5.9, females 7.9.
- External, Soft tissue and Skeletal abnormalities: No treatment related effects. Data not presented.

Source: Nelson et al. 1990
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS
Groups of approximately 15 female pregnant Sprague-Dawley rats with a mean maternal weight of 257 g at the beginning of pregnancy.

ADMINISTRATION / EXPOSURE
- Type of exposure: Inhalation, concentrations monitored continuously and recorded hourly.
- Duration of test/exposure: 7 hours a day from day 1-19 of gestation.
- Dose level: 0.4 mg/l which was the highest atmospheric concentration which could be generated at a temperature below 80F. Control animals were sham exposed.

MATING PROCEDURES: Sperm positive females used, no other information.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily for 1st week then weekly
- Food & water consumption: Weekly on days 7, 14 and 20.
- Clinical observations: Assume daily frequency not actually reported.
- Examination of uterine content: Gestation day 20 ovaries also removed with uterus for examination of corpora lutea, implantations, resorption sites and live foetuses recorded.
- Examination of fetuses: Gestation day 20 examined for external, visceral and skeletal anomalies. Foetal weights and sex were recorded.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
Not carried out.

STATISTICAL METHODS: Multivariate analysis of variance (MANOVA) and ANOVA. Foetal incidence data were analysed using the Variance Test for Homogeneity of the Binomial Distribution or ANOVA. The Kruskal-Wallis test was used if a non-parametric analysis was more appropriate.

Conclusion: The NOAEL for maternal toxicity, foetotoxicity and teratogenicity in rats following inhalation exposure to n-octanol during gestation (Gestation days 1-19) is >0.4 mg/l (the highest attainable concentration). There were no adverse effects on any of the maternal or foetal parameters investigated.
Cited in Iuclid 2000.

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: Iuclid 2000 European Commission - European Chemicals Bureau Octan-1-ol Cas# 111-87-5

Nelson, B.K., Brightwell, W.S., Khan, A., Krieg, Jr., E.F., and Hoberman, A.M. 1990. Developmental toxicology assessment of 1-octanol, 1-nonanol, and 1-decanol administered by inhalation to rats. J. Am. Coll. Toxicol. 9:93-97.

Nelson, B.K; Brightwell, W.S; Kreig, E.F. 1996 Developmental toxicology of industrial alcohols: A summary of 13 alcohols administered by inhalation to rats. Tox. Ind. Hlth. 6(3/4): 373-387.

11-MAY-2006 (62) (83) (84)

<u>1-Octanol (111-07-5) for 1-Octanol Aluminum Salt (14624-13-6)</u>

Species: other: Chick embryo **Sex:**
Route of administration: other: Injected suprablastodermically
Frequency of treatment: once
Doses: 0.05M
Control Group: other: olive oil

Method: other: see text
Year: 1979

GLP: no data
Test substance: > 90% 1-octanol (111-87-5)

Result: N-octanol showed no significant teratological potential compared to the control group. Malformations were observed in 6.45% of the n-octanol treated embryos vs 7.9% of the controls.
Source: Forschmidt et al. 1979
Hayes Consultancy Service Bromley, Kent
Test condition: Very little experimental detail available in the abstract report of this study. Up to 50 chick embryos were injected at 72 hours of incubation. The potential teratogenic effectof the test material on the embryos was compared to a solvent control group (olive oil).
Reliability: (4) not assignable
Abstract
Reference: Forschmidt, P., Liban, E., and Abramovici, A. 1979. Teratogenic activity of flavor additives. Teratology 19(2):26A. (Abstract).
15-SEP-2004 (41)

1-Decanol (112-30-1) for 1-Decanol Aluminum Salt (26303-54-8)

Species: rat **Sex:** female
Strain: Sprague-Dawley
Route of administration: inhalation
Exposure period: 19 days
Frequency of treatment: 7-hours/day
Duration of test: 20 days
Doses: 100 mg/m3
Control Group: yes
NOAEL Maternal Toxity: > .1 mg/l
NOAEL Teratogenicity: > .1 mg/l

Method: other
Year: 1990
GLP: no data
Test substance: > 90% 1-decanol (112-30-1)
Result: NOAEL : 0.1 mg/l for maternal and foetal toxicity. No evidence of maternal toxicity, foetotxicity or teratogenicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: Within 5-10% of the nominal concentration of 0.1 mg/l when measured by Infrared analysis. This is the highest attainable dose under the conditions of the study. Actual dose achieved 0.1 mg/l.

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: Not reported
- Number aborting: Not reported
- Number of resorptions: Comparable in treated and control groups. Mean resorptions/litter control 0.5, treated 0.5.
- Number of corpora lutea: Comparable between treated and control groups. Mean corpora lutea/litter control 14.9, treated 13.8.
- Duration of Pregnancy: Not reported.
- Body weight: Weight gain was comparable in treated and control groups.
- Food/water consumption: Comparable between treated and control groups.
- Description, severity, time of onset and duration of clinical signs: None
- Hematological findings incidence and severity: Not carried out.
- Clinical biochemistry findings incidence and severity: Not carried out.
- Gross pathology incidence and severity: Not carried out.
- Organ weight changes: Not carried out.
- Histopathology incidence and severity: Not carried out.

FETAL DATA:
- Litter size and weights: Comparable between treated & control groups. Litter size (mean) control 13.5, treated 13,1.
- Sex ratio: No significant difference between treated and controls. Controls/litter (mean) male 6.6, female 6.9; Treated/litter (mean) male 6.8, female 6.3.
- External, Soft tissue and Skeletal abnormalities: No treatment related effects.

Source: Nelson et al. 1990.
Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS
Groups of approximately 15 female pregnant Sprague-Dawley rats with a mean maternal weight of 281 g at the beginning of pregnancy.

ADMINISTRATION / EXPOSURE
- Type of exposure: Inhalation, concentrations monitored continuously and recorded hourly.
- Duration of test/exposure: 7 hours a day from day 1-19 of gestation.
- Dose level: 0.1 mg/l which was the highest atmospheric concentration which could be generated at a temperature below

80F.
- Control group: The treated animals were compared with pooled controls from 11 studies using the same protocol conducted over a 5 year period.
MATING PROCEDURES: Sperm positive females used, no other information.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily for 1st week then weekly
- Food & water consumption: Weekly on days 7, 14 and 20.
- Clinical observations: Assume daily frequency not actually reported.
- Examination of uterine content: Gestation day 20 ovaries also removed with uterus for examination of corpora lutea, implantations, resorption sites and live foetuses recorded.
- Examination of fetuses: Gestation day 20 examined for external, visceral and skeletal anomalies. Foetal weights and sex were recorded.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
Not carried out.

STATISTICAL METHODS: Multivariate analysis of variance (MANOVA) and ANOVA. Foetal incidence data were analysed using the Variance Test for Homogeneity of the Binomial Distribution or ANOVA. The Kruskal-Wallis test was used if a non-parametric analysis was more appropriate.

Conclusion: The NOAEL for maternal toxicity, foetotoxicity and teratogenicity to rats following inhalation exposure to n-decanol during gestation (Gestation days 1-19) is 0.1 mg/l (the highest attainable concentration). There were no adverse effects on any of the maternal or foetal parameters investigated.

Reliability: (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: HSDB, 2004 on line.

Nelson, B.K., Brightwell, W.S., Khan, A., Krieg, Jr., E.F., and Hoberman, A.M. 1990. Developmental toxicology assessment of 1-octanol, 1-nonanol, and 1-decanol administered by inhalation to rats. J. Am. Coll. Toxicol. 9:93-97.

Nelson, B.K; Brightwell, W.S; Kreig, E.F. 1996 Developmental toxicology of industrial alcohols: A summary of 13 alcohols administered by inhalation to rats. Tox. Ind. Hlth. 6(3/4): 373-387

RTECS on line 2004 Decyl Alcohol.

11-MAY-2006 (46) (64) (65) (74)

1-Dodecanol (112-53-8) for 1-Dodecanol Aluminum Salt (14624-15-8)

Species	:	rat
Sex	:	female
Strain	:	Wistar
Route of admin.	:	oral feed
Exposure period	:	Up to 54 days, premating, mating and gestation until post natal day 5.
Frequency of treatment	:	continuous in diet
Duration of test	:	up to 54 days
Doses	:	0, 100, 500, 2000 mg/kg bw/day
Control group	:	yes
NOAEL Maternalt.	:	= 2000 mg/kg bw
NOAEL Teratogen	:	= 2000 mg/kg bw
Method	:	other: Combined repeat dose and reproductive/developmental toxicity Screening Test
Year	:	1992
GLP	:	yes
Test substance	:	dodecanol (112-53-8)
Test substance	:	other TS: Dodecanol (112-53-8) Purity >99%
Test condition	:	Groups of 12 female rats were given dodecanol in the diet at doses of 0, 1500 ppm, 7500 ppm, and 30000 ppm (0, 100, 500 and 2000 mg/kg/day) for a period of 14 days prior to mating then throughout mating and gestation until post natal day 5 when dams and offspring were sacrificed. This is part of a combined repeat dose and reproductive/ developmental screening study (guideline draft OECD 422) Reproductive parameters examined were pregancy rate, length of gestation, implantations, corpora lutea and resorptions. On post natal day 5 the pups were weighed and examined macroscopically for external malformations then sexed and examined for internal malformations. For full details of this study see chapter 5.4 Repeated dose toxicity and chapter 5.8.1 Fertility
Result	:	NOAEL: 2000 mg/kg/day (highest dose tested) for systemic and reproductive toxicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: ca 100, 500 and 2000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Parental data:
- Body weight: No treatment related effects.
- Food/water consumption: No treatment related effects.
- Description, severity, time of onset and duration of clinical signs: None reported.
- Pregancy rate: There was no statistically significant difference in pregancy rates although they were reduced in treated groups C 92%, 100 & 500 mg/kg 83%, 2000 mg/kg/day 75% these were within the normal historical control range according to the authors (actual historical control data not presented). Lack of statistical significance confirmed using Qui2-test.
- Fertility index: Not reported
- Precoital interval: Not reported
- Duration of gestation: Comparable in treated and control dams (23 days in all groups).
- Gestation index: Not reported
- Changes in lactation: Not reported
- Changes in estrus cycles: Not reported
- Mortality: None
- Number of implantations: No significant differences in the numbers of implantations between treated and control groups (mean 13 in control group, 14 in each treated group).. There were no resorptions.
- Number of corpora lutea: No significant differences between treated and control groups.
- Ovarian primordial follicle counts: Not reported
- Foetal toxicity:
- Litter size and weights: No effect of treatment. Litter size mean Controls 13.25, low dose 13.27, mid dose 13.2, high dose 13.33. Mean litter weights at day 1 were 75, 75, 71 and 77 gm and at day 4 106, 107, 101 and 104 gm for control, low, mid and high dose respectively. No statistical significance.
- Sex and sex ratios: No treatment related effects.
- Post natal survival until day 5: Similar in treated and control groups.
- Foetal anomalies: There were no treatment related changes in the incidence of external or visceral malformations visible on macroscopic examination.

Conclusion : Development was assessed as part of a combined repeat dose and reproductive/developmental toxicity study. There were no adverse effects on maternal toxicity or reproductive parameters and no adverse effect on the offspring which were examined on postnatal day 5. The NOAEL for maternal and foetotoxicity was 2000 mg/kg/day in

rats receiving dodecanol in the diet for up to 54 days (premating, mating, gestation to postnatal day 5). There was no evidence of teratogenicity from the limited examinations of the pups which were carried out.

Reliability : (1) valid without restriction
Comparable to guideline study (draft guideline) with acceptable restrictions

Source : Hansen 1992a.
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Hansen, E. 1992a. Combined repeat dose and reproductive/developmental toxicity screening test on 1-dodecanol in rats. Institut of Toxicology, Danish National Food Agency, IT 921105.

11.08.2005 (9)

1-Tetradecanol (112-72-1) for 1-Tetradecanol Aluminum Salt (67905-32-7)

Remark: Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that tetradecanol is not expected to be a developmental toxicant in the absence of maternal toxicity.

Source: Hayes Consultancy Service Bromley, Kent

Test substance: > 95% 1-Tetradecanol (112-72-1)

Conclusion: Not expected to be a developmental toxicant in the absence of maternal toxicity.

Reliability: (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic

Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category
15-SEP-2005 (66) (67) (78)

1-Hexadecanol (36653-82-4) for 1-Hexadecanol Aluminum Salt (1914182-3)

Remark: Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that hexadecanol is not expected to be a developmental toxicant in the absence of maternal toxicity.
Test substance: >= 95% 1-hexadecanol (36653-82-4)
Conclusion: Not expected to be a developmental toxicant in the absence of maternal toxicity.
Reliability: (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
Reference: SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category.
25-OCT-2005 (80) (81) (94)

1-Octadecanol (112-92-5) for 1-Octadecanol Aluminum Salt (3685-81-7)

Species	:	Rat
Sex	:	Female
Strain	:	Wistar
Route of admin.	:	oral feed
Exposure period	:	Up to 54 days, premating, mating and gestation until post natal day 5.
Frequency of treatment	:	continuous in diet
Duration of test	:	Up to 54 days
Doses	:	0, 100, 500, 2000 mg/kg/bw/day
Control group	:	Yes
NOAEL Maternalt.	:	= 2000 mg/kg bw
NOAEL Teratogen	:	= 2000 mg/kg bw
Method	:	other: Combined repeat dose and reproductive/developmental toxicity screening test
Year	:	1992
GLP	:	Yes
Test substance	:	octadecanol (112-92-5)
Test substance	:	Octadecanol (112-92-5) Purity 99%
Test condition	:	Groups 12 female rats were given otadecanol in the diet at doses of 0, 1500 ppm, 7500 ppm, and 30000 ppm (0, 100, 500 and 2000 mg/kg/day) for a period of 14 days prior to mating then throughout mating and gestation until post natal day 5 when dams and offspring were sacrificed. This is part of a combined repeat dose and reproductive/developmental screening study (similar to OECD 422). Reproductive parameters examined were pregancy rate, length of gestation, implantations, corpora lutea and resorptions. On post natal day 5 the pups were weighed and examined macroscopically for external malformations then sexed and examined for internal malformations. For full details of this study see chapter 5.4 Repeated dose toxicity and chapter 5.8.1 Fertility.
Result	:	NOAEL: 2000 mg/kg/day (highest dose tested) for systemic and reproductive toxicity. ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: ca 100, 500 and 2000 mg/kg/day TOXIC RESPONSE/EFFECTS BY DOSE LEVEL: - Parental data: - Body weight: No treatment related effects. - Food/water consumption: No treatment related effects. - Description, severity, time of onset and duration of clinical signs:

None reported.
- Pregnancy rate: There was no statistically significant difference (confirmed using a Qui2-test) in pregnancy rates although they were reduced in treated groups C 92%, 100 & 500 mg/kg 75%, 2000 mg/kg/day 67% these were within the normal historical control range according to the authors (actual historical control data not presented).
- Fertility index: Not reported
- Precoital interval: Not reported
- Duration of gestation: Comparable in treated and control dams.
- Gestation index: Not reported
- Changes in lactation: Not reported
- Changes in estrus cycles: Not reported
- Mortality: None
- Number of implantations: No significant differences in the numbers of implantations between treated and control groups. (Mean 13 in controls and low dose, 15 in mid and high dose groups). Resorptions mean for controls and low dose 0, for mid and high dose 1)..
- Number of corpora lutea: No significant differences between treated and control groups (mean controls 13, low and mid dose 14, high dose 15).
- Ovarian primordial follicle counts: Not reported
- Foetal toxicity:
- Litter size and weights: No effect of treatment. (mean litter size 11.73, 10.0, 13.6 and 13.38 for controls, low, mid and high dose respectively). Litter weights day 1 mean 69, 61, 75 and 75 gm; Day 4 mean 96, 84, 101 and 101gm for controls, low, mid and high dose respectively)

- Sex and sex ratios: No treatment related effects.
- Post natal survival until day 5: Similar in treated and control groups.
- Foetal anomalies: There were no treatment related changes in the incidence of external or visceral malformations visible on macroscopic examination.

Conclusion : Development was assessed as part of a combined repeat dose and reproductive/developmental toxicity study. There were no adverse effects on maternal toxicity or reproductive parameters and no adverse effect on the offspring which were examined on postnatal day 5. The NOAEL for maternal and foetotoxicity in rats, receiving octadecanol in the diet for up to 54 days (premating, mating, gestation until postnatal day 5), was 2000 mg/kg/day (highest dose level). There was no evidence of teratogenicity from the limited examinations of the pups which were carried out.

Reliability : (1) valid without restriction
Comparable to guideline study (draft guideline) with acceptable

restrictions

Source : Hansen 1992b.
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference Hansen, E. 1992b. Combined repeat dose and reproductive/developmental toxicity screening test on 1-octadecanol in rats. Denmark: Institute of Toxicology, National Food Agency, IT 911130.

08.01.2006 (9)

1-Eicosanol (629-96-9) for 1-Eicosanol Aluminum Salt (67905-31-1)

Remark: Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that eicosanol is not expected to be a developmental toxicant in the absence of maternal toxicity.

Test substance: >= 90% 1-eicosanol (629-96-9)

Conclusion: Not expected to be a developmental toxicant in the absence of maternal toxicity.

Reliability: (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

Reference: SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

15-SEP-2005 (18) (23)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Species: rat **Sex:** female

Strain: Sprague-Dawley

Route of administration: gavage
Exposure period: For 15 days prior to mating, during mating and up to Day 17 of gestation.
Frequency of treatment: daily
Duration of test: 20th day of gestation
Doses: 10, 100, 1000 mg/kg bw
Control Group: yes
NOAEL Maternal Toxity: = 1000 mg/kg bw
NOAEL Teratogenicity: = 1000 mg/kg bw

Method: other
Year: 2000
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)

Result: All female rats survived to sacrifice and no maternal toxicity was observed. The were no differences between treated and control animals in any of the rerpoductive endpoints investigated (corpora lutea, pre & post implantation sites, early & late resorption sites). The litter size, foetal weight and sex ratio observed in treated groups was comparable to the control group. There were no unusual macroscopic findings among foetuses. Microscopic examination did not show any increased incidence of anomalies in skeletal or soft tissues. See above chapter 5.8.1 for further details.
Source: Iglesias, 2002b
Hayes Consultancy Service Bromley, Kent
Test condition: This study was part of a reproductive/development study in rats. The study is fully reported in Chapter 5.8.1 Fertility. Female rats, 5-6 weeks of age received 0, 10, 100 or 1000 mg/kg bw of behenyl alcohol by gavage as an aqueous suspension with a constant dosing volume of 5 ml/kg. The females were mated to treated males. Females received the the test material for 15 days prior to mating, throughout mating and up to Day 17 of gestation. Reproductive endpoints were evaluated at day 20 of gestation were corpora lutea, pre & post implantation sites, early & late resorption sites, viable foetuses, position of foetuses in uterine horns. In addition, foetuses were weighed and examined for abnormalities. The neck, thoracic and abdominal cavities were examined and a microscopic skeletal examination was performed. Statistical analyses were performed on all endpoints.
Test substance: C22 alcohol CAS RN 661-19-8
Conclusion: 1000 mg/kg/day is the NOAEL for maternal toxicity, teratogenicity and foetotoxicity in rats receiving behenyl alcohol by gavage for 15 days premating, during mating and up until gestation day 17. This is based on the absence of

adverse effects in any of the parental, reproductive or foetal parameters examined.

Reliability: (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).

Flag: Critical study for SIDS endpoint

Reference: Iglesias, G, JJ Hlywka, JE Berg, MH Khalil, LE Pope and D Tamarkin. 2002b. The toxicity of behenyl alcohol: II. Reproduction studies in rats and rabbits. Regulatory Tox. and Pharm. 36, 80-85.

11-MAY-2006 (16)

1-Docosanol (661-19-8) for 1-Docosanol Aluminum Salt (67905-30-0)

Species: rabbit **Sex:** female
Strain: New Zealand white
Route of administration: gavage
Exposure period: days 6-19 of gestation
Frequency of treatment: daily
Duration of test: 28 days
Doses: 125, 500, 2000 mg/kg bw
Control Group: yes
NOAEL Maternal Toxity: > 2000 mg/kg bw
NOAEL Teratogenicity: > 2000 mg/kg bw

Method: other: ICH Harmonized Tripartite Guideline for Detection of Toxicity to Reproduction for Medicinal Products
Year: 2000
GLP: yes
Test substance: >95% 1-docosanol (661-19-8)

Result: NOAEL: 2000 mg/kg/day for maternal and foetal effects.

ACTUAL DOSE RECEIVED: 0, 125, 500, 2000 mg/kg/day

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: 20 (controls and top dose), 19 (125 and 500 mg/kg/day)
- Number aborting/total litter loss: A total of 3 females, one each in the control group and the 125 and 500 mg/kg groups were observed to have a total litter loss, the uterus of each female revealed early resorptions.
- Number of resorptions: Comparable to controls. Total resorptions (mean) 1.3, 1.3, 1.7 and 1.6; Early resorptions 0.4, 0.3, 0.4 and 0.7; Late resorptions 1.0, 1.1, 1.2, 0.9 for controls, low, mid and high dose groups respectively.

- Number of implantations: Comparable to controls.
- Pre and post implantation loss: Comparable to controls. Implantation loss pre 10.4, 14.2, 13.9 and 13.5%; Post 12.1, 12.0, 15.2, 14.7 for controls, low, mid and high dose groups respectively.
- Number of corpora lutea: Comparable to controls. Mean Corpora lutea 12.8, 12.9, 12.6 and 12.2 for controls, low, mid and high dose groups respectively.
- Duration of Pregnancy: Comparable to controls.
- Body weight, food/water consumption: Comparable to controls.
- Description, severity, time of onset and duration of clinical signs: The only clinical observations were of pale faeces in most females at the top dose level attributed to the presence of unabsorbed behenyl alcohol in the gastro-intestinal tract.

FETAL DATA:
- Litter size and weights, Number viable, Sex ratio: Comparable to controls. Viable young total 10.1, 9.8, 9.3 and 9.0 for controls, low, mid and high dose groups respectively.
- Anomalies: Macroscopic, visceral and skeletal examination of the foetuses revealed no variations which were outside the historical control incidence. Actual data were not reported.

Source: Iglesias, 2002b

Hayes Consultancy Service Bromley, Kent

Test condition: TEST ORGANISMS

Groups of 22 female New Zealand White rabbits aged ca 20-28 weeks at initiation (weight 3.29 - 4.98 kg)

ADMINISTRATION / EXPOSURE
- Type of exposure: gavage
- Duration of test/exposure: Days 6-19 of gestation
- Control group and treatment: vehicle control
- Vehicle: 1% aqueous Tween 80
- Concentration in vehicle: 20%
- Total volume applied: 10 ml/kg for top dose and controls, 0.625 and 2,5 ml/kg for the 125 and 500 mg/kg dose level respectively.
- Doses: 0 125, 500 and 2000 mg/kg behenyl alchol.

MATING PROCEDURES: Mated with proven fertile males then injected with luteinizing hormone to ensure ovulation.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain and water consumption: Daily
- Food consumption: Days 1-5, 6-12, 13-19, 20-23 and 24-28 inclusive.

- Clinical observations: Daily
- Examination of uterine content: On gestation day 29, pre and post-implantation sites, early & late resrption sites, viable foetuses and distribution in uterine horn. The ovaries were examined for numbers of coprora lutea.
- Examination of fetuses: Foetal and placental weights were recorded. All foetuses were examined macroscopically for abnormalities. All foetuses were subjected to visceral examination microscopically and stained for skeletal examination. The heads of 1/3 of the foetuses were also sectioned and examined.

STATISTICAL METHODS: STATISTICAL METHODS: one way analysis of variance and T-test on body weights, food & water consumption. Organ weights - Dunnetts or Behren's-Fischer's test. Nested analysis of variance and weighed t-test for foetal and placental weights.

Test substance: C22 alcohol CAS RN 661-19-8

Conclusion: The NOAEL for maternal toxicity, teratogenicity and foetotoxicity in rabbis, receiving C22 alcohol by gavage on gestation days 6-19, is 2000 mg/kg/day (top dose level). This is based on lack of statistically significant effects in the maternal, reproductive and foetal parameters evaluated at any dose level.

Reliability: (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).

Flag: Critical study for SIDS endpoint

Reference: Iglesias, G, JJ Hlywka, JE Berg, MH Khalil, LE Pope and D Tamarkin. 2002b. The toxicity of behenyl alcohol: II. Reproduction studies in rats and rabbits. Regulatory Tox. and Pharm. 36, 80-85.

11-MAY-2006 (16)

<u>1-Tetracosanol, 1-Hexacosanol, 1-Octacosanol, and 1-Triacontanol for their respective Aluminum Salts</u>

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	gestation days 6-15
Frequency of treatment	:	daily
Duration of test	:	day 20
Doses	:	100, 320, 1000 mg/kg bw
Control group	:	yes, concurrent vehicle

NOAEL Maternalt.	:	= 1000 mg/kg bw
NOAEL Teratogen	:	= 1000 mg/kg bw
Method	:	other: see text
Year	:	1998
GLP	:	no data
Test substance	:	C24-34 alcohols

Test substance : A C24-C34 alcohol, called D-002, the components of which are primarily isolated and purified from beeswax. The composition was C24 (13.2%), C26 (15.3%), C28 (17.5%), C30 (26.6%), C32 (17%), C34 (2.2%) and 7% "other well known, non-active substances". C24-34 even alcohols (D-002)

Test condition : TEST ORGANISMS Groups of 25 presumed pregnant females weight 175-204 g.

ADMINISTRATION / EXPOSURE
- Type of exposure: gavage on gestation days 6-15
- Duration of test/exposure: 20 days
- Treatment: 0, 100, 320 and 1000 mg/kg/day
- Control group and treatment: Concurrent, 10 mg/ml gum acacia suspension.
- Vehicle: 10 mg/ml gum acacia
- Concentration in vehicle: Variable to give a constant dosing volume.
- Total volume applied: 2 ml/kg

MATING PROCEDURES: 2 females to 1 male

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily
- Food consumption: Not reported.
- Clinical observations: Daily
- Examination of uterine content: Day 20, numbers of implants, resorptions and dead foetuses were recorded. The ovaries were examined for numbers of corpora lutea. Uteri of apparently non-pregnant animals were examined for evidence of implantation.
- Examination of fetuses: All live foetuses were examined externally and half were examined viscerally the other half for skeletal anomalies.

STATISTICAL METHODS: Maternal and foetal weights analyses by parametric analysis of variance followed by the Tukey test. Reproductive parameters were examined by the Kruskall-Wallis test. The incidence of malformations and skeletal variations was carried out using the Fischer exact test.

Result : NOAEL: 1000 mg/kg/day for maternal toxicity, foetotoxicity and teratogenicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 100, 320 and 1000 mg/kg/day

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: 21 controls, 19 at 100 mg/kg/day, 22 at 320 and 1000 mg/kg/day
- Number aborting: None
- Number of resorptions, implantations, pre and post implantation loss: Comparable in treated and control groups. No Implantation sites mean 10.1, 9.2, 10.8 and 10.1; % resorptions (early) 4, 1, 2 and 4 for controls, low, mid and high dose respectively.
- Number of corpora lutea: Comparable in treated and control groups. Mean corpora lutea 11.6, 11.8, 12.4 and 11.5 for controls, low, mid and high dose respectively.
- Body weight: No statistical differences between treated and control groups.
- Description, severity, time of onset and duration of clinical signs: None observed.

FOETAL DATA:
- Litter size and weights, number viable, sex ratio: No statistically significant differences between treated and control groups. Number of live foetuses mean 9.9, 8.9, 10.7 and 9.9; mean foetal weight 3.8, 4.0, 3.8 and 4.1 gm; Sex ratio male/female 1.22, 0.8, 1.26 and 1.13 for controls, low, mid and high dose respectively.
- External abnormalities: A single foetus with exencaphaly in the controls none in the treated group.
- Soft tissue abnormalities: None
- Skeletal abnormalities: Foetuses with supernumary or rudimentary ribs and retarded, rudimentary or asymmetrical ossification of the sternal centrum were observed in all treated and control groups the incidence was comparable between treated and control groups and without statistical significance. Incidence of foetuses with variations 10, 8, 13 and 6% for controls, low, mid and high dose groups respectively.

Conclusion : The NOAEL for maternal toxicity, teratogenicity and foetotoxicity in rats receiving C24-34 alcohol on gestation days 6-15 is 1000 mg/kg, the highest dose level tested. This is based on a lack of adverse effects in any of the parameters of maternal, reproductive or foetal toxicity investigated.

Reliability	:	(2) valid with restrictions Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment.
Source	:	Rodriguez, 1998 Hayes Consultancy Service Bromley, Kent
Flag	:	Critical study for SIDS endpoint
Reference		Rodriguez, MD, R Gamez, M Sanchez and H Garcia. 1998. Developmental Toxicity of D-002 (a Mixture of Aliphatic Primary Alcohols) in Rats and Rabbits. Journal of Applied Toxicology, 18, 313-316.
24.01.2005		(8)

1-Tetracosanol, 1-Hexacosanol, 1-Octacosanol, and 1-Triacontanol for their respective Aluminum Salts

Species	:	rabbit
Sex	:	female
Strain	:	New Zealand white
Route of admin.	:	gavage
Exposure period	:	day 6-18 of gestation
Frequency of treatment	:	daily
Duration of test	:	29 days
Doses	:	100, 320 and 1000 mg/kg bw
Control group	:	yes, concurrent vehicle
NOAEL Maternalt.	:	> 1000 mg/kg bw
NOAEL Teratogen	:	> 1000 mg/kg bw
Method	:	other: see text
Year	:	1998
GLP	:	no data
Test substance	:	C24-34 alcohols
Test substance	:	A C24-C34 alcohol, called D-002, primarily isolated and purified from beeswax. The composition is C24 (13.2%), C26 (15.3%), C28 (17.5%), C30 (26.6%), C32 (17%), C34 (2.2%) and 7% of "other well known, non-active substances". C24-34 even alcohol (D-002)
Test condition	:	TEST ORGANISMS Groups of 16-20 presumed pregnant females weight 2.5-3.5 kg. ADMINISTRATION / EXPOSURE - Type of exposure: gavage on gestation days 6-15 - Duration of test/exposure: 29 days - Treatment: 0.100, 320 and 1000 mg/kg/day - Control group and treatment: Concurrent, 10 mg/ml gum acacia suspension.

- Vehicle: 10 mg/ml gum acacia
- Concentration in vehicle: Variable to give a constant dosing volume.
- Total volume applied: 2 ml/kg

MATING PROCEDURES: Mated with males of the same breed until copulation was opbserved

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily
- Food consumption: Not reported.
- Clinical observations: Daily
- Examination of uterine content: Day 20, numbers of implants, resorptions and dead foetuses were recorded. The ovaries were examined for numbers of corpora lutea. Uteri of apparently non-pregnant animals were examined for evidence of implantation.
- Examination of fetuses: All live foetuses were examined externally and for visceral and skeletal anomalies.

STATISTICAL METHODS: Maternal and foetal weights analyses by parametric analysis of variance followed by the Tukey test. Reproductive parameters were examined by the Kruskall-Wallis test. The incidence of malformations and skeletal variations was carried out using the Fischer exact test.

Result : NOAEL: 1000 mg/kg/day for maternal toxicity, teratogenicity and foetotoxicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 100, 320 adn 1000 mg/kg/day

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: 20 controls, 16 at 1000 mg/kg/day, 17 at 320 mg/kg/day, 19 at 1000 mg/kg/day
- Number aborting: None
- Number of resorptions & implantations, pre and post implantation loss, number of corpora lutea: Comparable in treated and control groups. Corpora lutea (mean) 7.6, 6.8, 7.4 and 7.1; Implantation sites (mean) 6.7; 5.9, 6.4 and 5.6; Resorptions 4, 2, 2 and 6%; Early resorptions 5, 0, 4 and 4%; Late resorptions 0, 4, 0 and 3% for controls, low, mid and high dose respectively.
- Duration of Pregnancy: Comparable in treated and control groups.
- Body weight: No statistically significant differences between treated and control groups.
- Description, severity, time of onset and duration of clinical signs:

None observed.

FETAL DATA:
- Litter size and weights, viability, sex ratio: no differences between treated and control groups. No of live foetuses (mean) 6.3, 5.8, 6.1 and 5.1; Mean foetal weight 29.3, 30.7, 32.8 and 33.7 gm; Sex ration male/female 1.05, 1.12, 1.42 and 1.58 for controls, low, mid and high dose respectively.
- External abnormalities: 1 control foetus with acephaly, At 320 mg/kg/day two foetuses from different litters had hemivertebra with fused thoracic ribs.
- Soft tissue abnormalities: None
- Skeletal abnormalities: All groups showed skeletal variation such as extra rib or a pair of ribs, retarded ossification of the sternum, cleaved and fused sternal centra. The incidence of these variations was not dose related. Incidence of foetuses with variations 50, 48, 41 and 51% for controls, low, mid and high dose respectively.

Conclusion : The NOAEL for maternal toxicity, teratogenicity and foetotoxicity is 1000 mg/kg, the highest dose level tested. This is based on a lack of adverse effects in any of the parameters of maternal, reproductive or foetal toxicity investigated.

Reliability : (2) valid with restrictions
Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment.

Source : Rodriguez, 1998
Hayes Consultancy Service Bromley, Kent

Flag : Critical study for SIDS endpoint

Reference
24.01.2005

Rodriguez, MD, R Gamez, M Sanchez and H Garcia. 1998. Developmental Toxicity of D-002 (a Mixture of Aliphatic Primary Alcohols) in Rats and Rabbits. Journal of Applied Toxicology, 18, 313-316.
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