AR201-13646B

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Data Set

Existing Chemical	:	ID: 131-11-3
CAS No.	:	131-11-3
EINECS Name	:	dimethyl phthalate
EINECS No.	:	205-011-6
TSCA Name	:	1,2-Benzenedicarboxylic acid, dimethyl ester
Molecular Formula	:	C10H10O4

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	16.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	16.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - low MW phthalates
Printing date	:	02.11.2001
Revision date	:	
Date of last Update	:	02.11.2001
Number of Pages	:	20
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the Low Molecular Weight Phthalate Esters subcategory. The subcategory includes the following two CAS numbers:131-11-3 and 84-66-2.

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate

esters in this subcategory, Low molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of <C3. The U.S. HPV chemicals, dimethyl (DMP) and diethyl (DEP) phthalate, are included in this subcategory. Low molecular weight phthalates are commonly used as solvents or in cellulose acetate polymers rather than as plasticizers for PVC. Their relatively higher volatility and water solubility give them properties different than other phthalate esters, some of which translate to different biological properties. In particular, these phthalates have greater aqueous solubility, resulting in a potential to cause acute toxic effects in aquatic organisms.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Basic industry: basic chemicals
Remark	:	Low molecular weight phthalates are commonly used as solvents or in cellulose acetate polymers rather than as plasticizers for PVC.

02.11.2001

2.1 MELTING POINT

Value : -23 - ° C
Decomposition : no at - ° C
Sublimation : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Melting point calculation seems to give erroneously high results for the phthalate esters
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (3) invalid
08.10.2001 (9)

Value : 5.5 - ° C
Sublimation :
Method :
Year :
GLP :
Test substance : no data
Remark : Literature review collecting data from a variety of sources.

Manufacturer's data or handbook value
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
14.12.2000 (13)

2.2 BOILING POINT

Value : 285 - ° C at 1013 hPa
Decomposition :
Method : other
Year :
GLP :
Test substance :
Remark : Manufacturer's data or handbook value
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (4) not assignable
13.12.2000 (5)

Value : 249 ° C at 1013 hPa
Decomposition :
Method : Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Year : 2000
GLP :
Test substance :
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
13.12.2000 (9)

2.4 VAPOUR PRESSURE

Value	:	.00263 - hPa at 25° C
Decomposition	:	no
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

18.06.2001 (4)

Value	:	.0387 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

08.10.2001 (9)

Value	:	.00237 - hPa at ° C
Remark	:	Literature review collecting data from a variety of sources.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (13)

2.5 PARTITION COEFFICIENT

Log pow	:	1.61 - at 25° C
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Literature review collecting data from a variety of sources.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (4)

Log pow	:	1.61 - at 25° C
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Literature review collecting data from a variety of sources.

Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
14.12.2000 (13)

Log pow : 1.66 - at 25° C
Method other (calculated)
Year : 2000
GLP :
Test substance :
Method : Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
14.12.2000 (9)

2.6.1 WATER SOLUBILITY

Value : - 1778 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other
Year :
GLP :
Test substance :
Method : Water solubility calculated using WSKOWN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
08.10.2001 (9)

Value : - 4200 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other
Year :
GLP :
Test substance :
Remark : Literature review collecting data from a variety of sources.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
08.10.2001 (13)

Value : - 5220 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other
Year :
GLP :
Test substance :
Method : Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions

13.12.2000 (4)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.0000000000005738 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

14.12.2000 (9)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	2.8 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

13.12.2000 (9)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	7.567
Water (level I)	:	88.8
Soil (level I)	:	3.593
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (8)

3.3.2 DISTRIBUTION

Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level I
Year	:	2000
Result	:	Soil - 3.593% Air - 7.567% Water - 88.8% Sediment - 0.80% Suspended sed. - 0.0025%
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (8)

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	domestic sewage
Concentration	:	20mg/l related to Test substance related to
Contact time	:	28 day
Degradation	:	= 85.9 - % after
Result	:	readily biodegradable
Deg. Product	:	
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA 1982, CO2 Evolution, Shake Flask (modified Gledhill). Inoculum-Domestic sewage, soil, and mineral medium. Kinetics-Not Reported Degradation Products-Not Reported Analytical Monitoring-Yes
Result	:	Concentrations-Nominal test concentration = 20mg/L for test substance and glucose. Units-% biodegradation Value->99% primary, and 85.9% (sd 12.2) ultimate biodegradation. Primary degradation is expressed as the loss of initial test substance. Ultimate biodegradation is expressed as the percentage of ThCO2 in each flask
Test condition	:	Test Conditions-Inoculum was aged for 2 weeks prior to test initiation. The test chemical was added to flasks containing medium and inoculum. The flask were incubated and shaken in the dark for 28 days. Three replicates for CO2 evaluation and 4 replicates for primary degradation were tested. The CO2 production was captured in barium hydroxide solution. Primary biodegradation was determined at the beginning, middle and end by GC FID of entire contents of one replicate. A glucose and blank were also tested.. 2L Erlenmeyer flasks were used as test vessels. The pH at initiation was 7.0 to 7.2. Test flasks were shaken at a rate of 120rpm at 22 +/- 2 deg C.
Test substance	:	Dimethyl phthalate (CAS# 131-11-3) (1,2,-benzenedicarboxylic acid, dimethyl ester)

Synonym: DMP

Conclusion : The substance is readily biodegradable using mixed populations of microorganisms,

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

29.11.2000 (14)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	m = 56 -
Method	:	other
Year	:	1982
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians. Statistical methods-Moving average angle, Probit or Bionomial concentration.
Result	:	Nominal test concentrations: control, 6.2, 12.0, 25.0, 50.0, and 100.0mg/L. Mean measured test concentrations: <0.036, 6.1, 10.0, 19.0, 38.0, and 83.0mg/L. Units-ppm Value-LC50=56.0 ppm Mean measured values used in calculation of LC50. Total mortality observed in both replicates of the high treatment (83mg/L) and one replicate of the middle treatment (19mg/L). Analytical samples taken at time zero and on a composite of replicates at termination. Measured values dropped slightly during the exposure period. Fish mean Total length=45mm, mean wet weight=0.76. Test temperature=12 +/- 1 Deg C., The pH range was 6.7 to 7.4. The mean Dissolved Oxygen ranged from 8.2 to 9.0mg/L. Fish were obtained from a Montana supplier.
Test condition	:	Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15L of solution. The diluter maintained a water turnover rate of 5-8 tank volumes per day. Two replicates of ten organisms were tested per treatment. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection.
Test substance	:	Dimethyl phthalate (CAS# 131-11-3) (1,2,-benzenedicarboxylic acid, dimethyl ester) Synonym: DMP
Conclusion	:	Test substance is toxic to fish below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document.1
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

08.10.2001 (2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
EC50	:	m = 45.9 -
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975, Statistical methods-Moving average angle, Probit or Bionomial Concentration.
Result	:	Nominal test concentrations: control, 39, 66, 110, 1800, 300 mg/L. Measured test concentrations: <0.007, 34, 52, 83, 170, 280/260 mg/L. (Day O). Measured concentrations <0.007, 13, 24, 36/48, 94, 180 mg/L (Day 2). Value- LC50=>52.0 ppm (based upon time zero analytical samples) Value recalculated as 45.9ppm as per USEPA current practices using mean of measured initiation and termination samples.1 Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined 33 to 62% during study exposure from all test solutions during the test.
Test condition	:	Test treatments were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 30 minutes. The stock solution was prepared at the highest treatment concentration. Dilutions of the stock were prepared for each treatment level. Three replicates of five organisms were tested per treatment. Test vessels were 250ml beakers with 200ml of test solution. Analytical method was Gas Liquid Chromatography (GLC). Test temperature=22 +/- 2 Deg C., The pH was 8.5 at initiation and ranged from 7.9 to 8.3 at Day 2. Dissolved Oxygen ranged from 7.8 to 8.6 at initiation and 6.0 to 8.2 at Day 2. Daphnia were <24 hours old and obtained from in-house stock. Nominal test concentrations: control, 39, 66, 110, 1800, 300mg/L. Measured test concentrations <0.007, 34, 52, 83, 170, 280/260mg/L (Day 0) Measured concentrations <0.007, 13, 24, 36/48, 94, 180mg/L (Day 2),
Test substance	:	Dimethyl phthalate (CAS# 131-11-3) (1,2,-benzenedicarboxylic acid, dimethyl ester) Synonym: DMP
Conclusion	:	Test substance is toxic to Daphnia below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document.1
Reliability	:	(2) valid with restrictions Reliability-Daphnids trapped at the surface in all exposure concentrations. Reliability-Daphnids trapped at the surface in all exposure concentrations.

Flag : Critical study for SIDS endpoint
08.10.2001 (1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint :
Exposure period : 6 day
Unit : mg/l
Analytical monitoring : yes
EC50 : m = 142 -
Method : other
Year : 1983
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Method : Method/Guideline-EPA 600/9-78-018, Printz Algal Assay Bottle Test, 1978.
Statistical methods-Moving average angle, Probit or Bionomial
Test type-Static Acute
Result : Concentrations-Nominal test concentrations: 62.5 125, 250, 500, 1000 ppm.
Measured test concentrations = 65.7, 141.3, 267.3, 544.7, 1409.4 ppm (Day 0),
Measured test concentrations = 63.7, 124.7, 317.8, 650.6, 1249.8 ppm (Day 6)

Units- mg/L
Value-EC50=145.6 ppm (95%CI 95.4 to 240.2)based upon Day 0 measured values only.
Value recalculated as 142.0 ppm as per USEPA current practices using mean of measured initiation and termination samples 1.

Lowest two concentrations showed stimulatory effect as compared to the control.
In-vivo chlorophyll a, measured daily until less than 5% change. Both cell numbers and in-vivo chlorophyll a, measured at termination.
Analytical samples taken at time zero and on a composite of replicates at termination.
Reliability-Control chlorophyll or cell counts not reported.
Test condition : Test substance was added to Algal Growth Medium equal to the highest test concentration (1000ppm) and stirred for one hour and settled for one-half hour. Fifty percent (50%) dilutions were made of this stock solution using algal growth media (dilution water and control) and tested. Initial algal concentration was 2.0x104 cells/ml. Lighting =4,3000lux, Test temperature=24+/-1 Deg C. The pH range was 7.0 at initiation and 7.6 - 8.3 at day 6. Algal culture stock obtained from Univ. of Texas at Austin.
Test substance : Dimethyl phthalate (CAS# 131-11-3)
(1,2,-benzenedicarboxylic acid, dimethyl ester)
Synonym: DMP
Conclusion : Test substance is toxic to algae below its water solubility level.
Data selected based upon routine species, measured data and representative value, as compared with those found in reference document 1.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
28.11.2000 (3)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	no data
Number of animals	:	40
Vehicle	:	other: Undiluted test material administered
Value	:	= 6900 - mg/kg bw
Method	:	other
Year	:	1948
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	There were no remarkable findings noted during the post-treatment observation period.
Test condition	:	Rats were fasted for 18 hours prior to receiving the test compound. The animals were observed for six days following dosing and all deaths were recorded. The dose levels of dimethyl phthalate used in this study were not specified. The material was administered in graded doses so that a dose-mortality curve could be determined. The LD50 was estimated from this dose-mortality curve.
Test substance	:	1,2-benzenedicarboxylic acid, dimethyl ester (dimethyl phthalate) CAS #: 131-11-3
Conclusion	:	Under the conditions of this study, dimethyl phthalate has a low order of acute oral toxicity in rats.
Reliability	:	(2) valid with restrictions Reliable with restrictions; insufficient data on the actual doses used.
Flag	:	Critical study for SIDS endpoint

31.10.2000 (6)

5.4 REPEATED DOSE TOXICITY

Species	:	rabbit
Sex	:	no data
Strain	:	
Route of admin.	:	dermal
Exposure period	:	90 days
Frequency of treatment	:	Not Specified
Post obs. period	:	Not Specified
Doses	:	Up to 4 ml/kg (>4 g/kg)
Control group	:	no data specified
Method	:	other
Year	:	1948
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Systemic effects observed at the highest dose level (4 ml/kg). Signs of toxicity included nephritis at the two higher dose levels; pulmonary edema and slight kidney damage. No evidence of dermatitis was observed.
Test condition	:	Limited data are available on the test conditions. Tissues collected from rabbits receiving the test material for 90 days were subjected to histopathological evaluations. Approximately 7000 individual tissues were examined.
Test substance	:	1,2-benzenedicarboxylic acid, dimethyl ester (dimethyl phthalate)

CAS #: 131-11-3

Conclusion : Based on the results of this study, it was concluded that the test material was safe for its recommended use.

Reliability : (2) valid with restrictions
Reliable with restrictions; limited detail regarding the experimental design and dose selection.

Flag : Critical study for SIDS endpoint

01.11.2000 (6)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium TA98; TA100; TA1535; TA1537
Concentration : 0, 33, 100, 333, 1,000, 2166, 3000, 3333, 5000, 6666 mg/plate
Cycotoxic conc. : 6666 mg/plate
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year : 1985
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Method : Metabolic activation: With and without S9 (metabolic activation enzymes and cofactors from Aroclor 1254-induced male Sprague-Dawley rat or Syrian hamster liver);

Statistical Methods: A positive response was defined as a reproducible, dose-related increase in histidine-independent colonies (revertants) in any one strain/activation combination. An equivocal response is defined as an increase in revertants which is not dose-related, not reproducible or is not of sufficient magnitude to support mutagenicity. A negative response is obtained when there is no increase in revertant colonies.

Result : Dimethyl phthalate was negative in all strains. The high dose of DMP (6666 mg/plate) was toxic to the bacteria.

Test condition : Dimethyl phthalate was incubated in the tester strains either in buffer or S9 mix for 20 minutes at 37°C. Top agar supplemented with l-histidine and d-biotin was added, and the contents of the tubes were mixed and poured onto the surfaces of minimal glucose agar plates. Histidine-independent mutant colonies arising on these plates were counted following incubation for 2 days at 37°C. Three replicates were used for each dose. Positive controls were as follows: Sodium azide (TA 1535, TA 100), 4-nitro-o-phenylenediamine (TA 98), 9-aminoacridine (TA 1537). Concurrent solvent and positive controls were included in all experiments. A preliminary range-finding study was used to determine the high dose level. This study was conducted with TA 100 in the presence and absence of S-9. A repeat assay was performed in order to verify the data produced in the initial assay.

Test substance : 1,2-benzenedicarboxylic acid, dimethyl ester (dimethyl phthalate)
CAS #: 131-11-3

Conclusion : No mutagenic activity was observed with dimethyl phthalate in Salmonella strains TA 98, TA 100, TA 1535 and TA 1537.

Reliability : (1) valid without restriction
Reliable without restrictions; NTP-sponsored study.

Flag : Critical study for SIDS endpoint

18.06.2001 (11)

Type : Chromosomal aberration test
System of testing : Chinese Hamster Ovary (CHO) cells

Concentration	:	10.5 hr incubation: 150, 498 and 1500 mg/ml 12.0 hr incubation: 498, 1500 and 4980 mg/ml 20.5 hour incubation: 3060, 4080 and 5100 mg/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 473 "Genetic Toxicology: In vitro Mammalian Cytogenetic Test"
Year	:	1987
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	With and without S9 (metabolic activation enzymes and cofactors from Aroclor 1254-induced male Sprague-Dawley rats); Statistical tests were performed on both the dose response curve and individual dose points. A statistically significant (P < 0.05) difference for one dose point and a significant trend (P < 0.015) were considered weak evidence of a positive response; significant differences for two or more doses indicate the trial is positive.
Result	:	Negative. No induction of chromosomal aberrations was observed in CHO cells in the presence or absence of S9.
Test condition	:	In the assay without S9, cells were incubated in McCoys 5A medium for 8.5 hours. Colcemid was added and incubation continued for 2 hours. Cells treated with S9 were treated with dimethyl phthalate for 2 hours, after which the treatment medium was removed and cells were then incubated for 10 hours in fresh medium. Colcemid was added during the final 2 hours of the incubation. Cell were selected for scoring based on good morphology and karyotype. Slides were scored blind and were read by the same person. DMSO was used as the solvent control at all incubation time points. Mitomycin-C was used as the positive control at 10.5 hours. Cyclophosphamide was used as the positive control at both 12.0 and 20.5 hours incubations. Two trials were conducted with S9, one using the standard 12 hour incubation while the second used a 20.5 hour incubation to ensure that CHO cells were exposed to DMP for at least one complete cell cycle.
Test substance	:	1,2-benzenedicarboxylic acid, dimethyl ester (dimethyl phthalate) CAS #: 131-11-3
Conclusion	:	Under conditions of this study, dimethyl phthalate was inactive in the chromosome aberration assay at doses up to 5100 mg/ml.
Reliability	:	(1) valid without restriction Valid without restrictions
Flag	:	Critical study for SIDS endpoint

18.06.2001 (10)

5.8 TOXICITY TO REPRODUCTION

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	Gestation days 6-15
Frequency of treatment	:	Daily
Duration of test	:	

Doses	:	0.0, 0.25, 1.0 or 5.0% (0, 0.20, 0.84, and 3.57 g/kg/day).
Control group	:	yes
NOAEL Maternalt.	:	= 840 - mg/kg bw
NOAEL Teratogen	:	> 3570 - mg/kg bw
Method	:	OECD Guide-line 414 "Teratogenicity"
Year	:	1993
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Statistical methods: ANOVA; Williams' and Dunnett's Multiple Comparison Test, Fisher's exact probability test
Result	:	The actual doses received were 0.20, 0.84 and 3.57 g/kg/day based on maternal body weights and food consumption. No dams died during gestation. Pregnancy rates were 89-93% for all treatment groups. Food consumption and body weight decreases were observed in animals in the 5.0% treatment groups. Relative kidney weight was increased in the high dose group. No histopathologic effects on the kidneys were observed in any of the treatment groups. In addition, there were no effects on the number of implantation sites, or percent resorptions. No effects on mean fetal body weight, viability, sex ration, or growth and development.
Test condition	:	After a 7 day quarantine period, breeding pairs were cohabited overnight. Gestation day 0 was determined the morning that vaginal sperm was found. Initial body weights of females were between 207- 273 grams. On gestation day 0, animals were randomly assigned to treatment groups consisting of 25-32 animals. Animals were weighed on the morning of gestation day 0, 3, 6, 9, 12, 15, 18 and 20. In addition, animals were observed daily for signs of toxicity. Animals were observed daily for overt signs of toxicity. On GD 20, animals were sacrificed and maternal body, liver, kidneys, and intact uterus were weighed. Fetuses were weighed, examined for external and visceral abnormalities.
Test substance	:	1,2-benzenedicarboxylic acid, dimethyl ester (dimethyl phthalate) CAS #: 131-11-3
Conclusion	:	Under the conditions of this study, DMP was not a selective developmental toxicant. DMP exposure was associated with maternal effects at the high dose level.
Reliability	:	(1) valid without restriction Reliable without restrictions; comparable to guideline study.
Flag	:	Critical study for SIDS endpoint

18.06.2001 (7)

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	i.p.
Exposure period	:	Gestation day 5, 10 and 15
Frequency of treatment	:	
Duration of test	:	
Doses	:	0, 0.33, 0.67, and 1.12 ml/kg (~0, 400, 800, 1300 mg/kg)
Control group	:	yes
Method	:	other
Year	:	1972
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Students t-test; Methods of Weil (1952) and Cornfield and Mantel (1950).
Result	:	Limited information on maternal effects (food consumption, body weight changes, deaths) were provided. At both the high and low dose levels, dimethyl phthalate produced an increase in the number of resorptions. Skeletal malformations included elongated and fused ribs, two fetuses did not have tail bones, and three had abnormal and incomplete skull bones. At the high dose, three fetuses

had neither tails nor eyes, one fetus had a normal tail but was without eyes.

Test condition : Female rats were selected after observation of at least two complete estrous cycles. The onset of gestation was determined by the presence of sperm in the vaginal smear and was recorded as Day 0. Dimethyl phthalate was administered to rats at doses representing one-tenth, one-fifth, and one-third of the acute LD50. On the day before parturition (day 20), each rat was sacrificed by an overdose of ether. Following sacrifice, the numbers of corpora lutea, resorption sites and viable and dead fetuses were recorded. Fetuses were also examined for skeletal malformation and variations.

Test substance : 1,2-benzenedicarboxylic acid, dimethyl ester (dimethyl phthalate)
CAS # 131-11-3

Conclusion : Although fetal data were provided, it is difficult to place these data into the proper context without information regarding toxic effects to the dams. Also, the conventional developmental toxicity study designed was not used.

Reliability : (3) invalid
Not reliable. Non-standard study design; insufficient data.

31.10.2000 (12)

(1) CMA Study, Acute Toxicity of Fourteen Esters to Daphnia magna., Springborn Bionomics, Inc. 1984. Report # BW-84-4-1567.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(2) CMA Study, Acute Toxicity of Fourteen Esters to Rainbow Trout Salmo gairdneri Under Flow-Through Conditions. EG&G Bionomics, Inc. 1983. Report # BW-83-3-1373, Performed Jul 1982 to Jan 1983.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(3) CMA Study, Toxicity of Fourteen Esters to the Freshwater Green Alga Selenastrum capricornutum. 1984. Study performed by Springborn Bionomics, Inc., 10 - 16 Sep 1982.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(4) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, chemosphere 41:1389-1399.

(5) David, R., R. McKee, J. Butala, R. Barter and M. Kayser (2001), Chapter 80 - Esters of Aromatic Mono, Di and Tricarboxylic acids and Di, Tri, or Polyalcohols, Patty's Toxicology, 5th edition, Vol 6., J Wiley & Sons, Inc. pp 635-932.

(6) Draize, J. H. (1948). Toxicological investigations of compounds proposed for use as insect repellants, A. Local and system effects following topical skin application. Acute oral toxicity. C. Pathological Examination", Journal of Pharmacology and Experimental Therapeutics 93:26-39.

(7) Field et al., (1993). Developmental toxicity evaluation of diethyl and dimethyl phthalate in rats. Teratology 38:33-44.

(8) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(9) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(10) NTP (1995). Toxicology and carcinogenesis studies of diethylphthalate in F344/N rats and B6C3F1 mice with dermal initiation/promotion study of diethylphthalate and dimethylphthalate in male Swiss CD-1 mice. NTP TR 429, NIH Publication No. 95-3356.

(11) NTP (1995). Toxicology and carcinogenesis studies of diethylphthalate in F344/N rats and B6C3F1 mice with dermal initiation/promotion study of diethylphthalate and dimethylphthalate in male Swiss Cd-1 mice. NTP TR 429, NIH Publication No. 95-3356.

(12) Singh et al (1972). Teratogenicity of phthalate esters in rats. Journal of Pharmaceutical Science 61:51-55.

(13) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997), the Environmental Fate of Phthalate Esters: A literature Review, Chemosphere 35:667-749.

(14) Sugatt, R.H. et al, 1983 Shake Flask Biodegradation of 14 Commercial Phthalate Esters. Syracuse Research Corporation, Syracuse, NY. SRC# L1543-05. Performed for CMA.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the Low Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There is a large amount of data for the physicochemical properties of dimethyl and diethyl phthalate. Computer models were also used to estimate these properties for comparison with measured values and additionally were used to predict environmental distribution.

A complete health effects SIDS data set is available for diethyl phthalate, and for dimethyl phthalate with the exception of adequate reproductive data. Both DMP and DEP show minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for developmental effects. Although adequate reproductive data are not available for DMP, data on DEP indicate that this material will not cause reproductive effects. This is further supported by data showing that neither DEP nor DMP had effects on male reproductive development. The lack of developmental effects observed with DMP, coupled with chronic toxicity studies showing no effects on reproductive organs, negates the need to conduct a reproductive study for DMP.

There are numerous published acute aquatic toxicity studies in a variety of species of fish, daphnia and algae for DMP and DEP. DMP and DEP are slightly soluble in aqueous systems. Acute effects on aquatic species are seen in the 10 to 100 ppm range.

02.11.2001

7.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 84-66-2
CAS No.	:	84-66-2
EINECS Name	:	diethyl phthalate
EINECS No.	:	201-550-6
TSCA Name	:	1,2-Benzenedicarboxylic acid, diethyl ester
Molecular Formula	:	C12H14O4

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	16.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	16.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - low MW phthalates
Printing date	:	02.11.2001
Revision date	:	
Date of last Update	:	02.11.2001
Number of Pages	:	23
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

20.10.2000

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the Low Molecular Weight Phthalate Esters subcategory. The subcategory includes the following two CAS numbers:131-11-3 and 84-66-2.

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Low molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of <C3. The U.S. HPV chemicals, dimethyl (DMP) and diethyl (DEP) phthalate, are included in this subcategory. Low molecular weight phthalates are commonly used as solvents or in cellulose acetate polymers rather than as plasticizers for PVC. Their relatively higher volatility and water solubility give them properties different than other phthalate esters, some of which translate to different biological properties. In particular, these phthalates have greater aqueous solubility, resulting in a potential to cause acute toxic effects in aquatic organisms.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Basic industry: basic chemicals
Remark	:	Low molecular weight phthalates are commonly used as solvents or in cellulose acetate polymers rather than as plasticizers for PVC.

02.11.2001

2.1 MELTING POINT

Value : -40 - ° C
Decomposition : no at - ° C
Sublimation : no
Method :
Year :
GLP :
Test substance :
Remark : Literature review collecting data from a variety of sources.
Manufacturer's data or handbook value
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
14.12.2000 (16)

Value : -1.7 - ° C
Decomposition : no at - ° C
Sublimation : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Melting point calculation by MBBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Melting point calculation seems to give erroneously high results for the phthalate esters
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (3) invalid
08.10.2001 (14)

2.2 BOILING POINT

Value : 298 - ° C at
Decomposition : no
Method : other
Year : 2000
GLP :
Test substance :
Remark : Manufacturer's data or handbook value
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (4) not assignable
02.11.2001 (8)

Value : 282 ° C at 1013 hPa
Decomposition :
Method : Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Year : 2000
GLP :
Test substance :
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
02.11.2001 (14)

2.4 VAPOUR PRESSURE

Value	:	.000648 - hPa at 25° C
Decomposition	:	no
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Decomposition	:	no
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (6)

Value	:	.00133 - hPa at 25° C
Decomposition	:	no
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Decomposition	:	no
Remark	:	Literature review collecting data from a variety of sources.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (16)

Value	:	.00668 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

08.10.2001 (14)

2.5 PARTITION COEFFICIENT

Log pow	:	2.38 - at 25° C
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Literature review collecting data from a variety of sources.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (16)

Log pow	:	2.54 - at 25° C
Method		other (measured)

Year	:	
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (6)

Log pow	:	2.65 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (14)

2.6.1 WATER SOLUBILITY

Value	:	184 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other: calculated
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

02.11.2001 (14)

Value	:	591 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (6)

Value	:	1100 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Remark	:	Literature review collecting data from a variety of sources.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (16)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.000000000003466 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	
Year	:	
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (14)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	2.9 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

14.12.2000 (14)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	10.4
Water (level I)	:	64
Soil (level I)	:	25.2
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000

14.12.2000 (13)

3.3.2 DISTRIBUTION

Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level I
Year	:	2000
Result	:	Soil - 25.2% Air - 10.4% Water - 63.8% Sediment - 0.561% Suspended sed. - 0.018%
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (13)

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	domestic sewage
Concentration	:	20mg/l related to related to
Contact time	:	28 day
Degradation	:	= 94.6 - % after
Result	:	readily biodegradable
Deg. Product	:	
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA 1982, CO2 Evolution, Shake Flask (modified Gledhill). Inoculum-Domestic sewage, soil, and mineral medium. Kinetics-Not Reported Degradation-Not Reported Analytical Monitoring-Yes
Result	:	Concentrations-Nominal test concentration = 20mg/L for test substance and glucose. Units-% biodegradation Value->99% primary, and 94.6% (sd 2.3) ultimate biodegradation. Primary degradation is expressed as the loss of initial test substance. Ultimate biodegradation is expressed as the percentage of ThCO2 in each flask.
Test condition	:	Test Conditions-Inoculum was aged for 2 weeks prior to test initiation. The test chemical was added to flasks containing medium and inoculum. The flask were incubated and shaken in the dark for 28 days. Three replicates for CO2 evaluation and 4 replicates for primary degradation were tested. The CO2 production was captured in barium hydroxide solution. Primary biodegradation was determined at the beginning, middle and end by GC FID of entire contents of one replicate. A glucose and blank were also tested.. 2L Erlenmeyer flasks were used as test vessels. The pH at initiation was 7.0 to 7.2. Test flasks were shaken at a rate of 120rpm at 22 +/- 2 Deg C.
Test substance	:	Diethyl phthalate (DEP CAS# 84-66-2) (1,2,-benzenedicarboxylic acid, diethyl ester) Synonym: DEP
Conclusion	:	The substance is readily biodegradable using mixed populations of

microorganisms,

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
29.11.2000 (17)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : flow through
Species : Salmo gairdneri (Fish, estuary, fresh water)
Exposure period : 120 hour(s)
Unit : mg/l
Analytical monitoring : yes
LC50 : m = 12 -
Method : other
Year : 1982
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Method : Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians.

Statistical methods-Moving average angle, Probit or Bionomial Concentration.

Result : Mean measured values used in calculation of LC50.
The 96 hour LC50 was identical to the 120 hour value.

Analytical samples taken at time zero and on a composite of replicates at termination. Measured values dropped slightly during the exposure period. The highest three test concentrations exhibited toxicity.

Fish mean Total length=45mm, mean wet weight=0.76g.

Concentrations-Nominal test concentrations: control, 2.5, 5.0, 10.0, 20.0 and 40.0 mg/L.

Mean measured test concentrations: <0.0067, 1.9, 3.8, 8.4, 16.0, and 33.0/L.

Units-ppm
Value-LC50=12.0 ppm

Test condition : Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15L of solution. The diluter maintained a water turnover rate of 5-8 tank volumes per day. Two replicates of ten organisms were tested per treatment. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection.

Test temperature=12 +/- 1 Deg C.

The pH range was 7.1 to 7.4.

The mean Dissolved Oxygen ranged from 8.6 to 9.5mg/L.
Fish were obtained from Montana.
Concentrations-Nominal test concentrations: control, 2.5, 5.0, 10.0, 20.0, and 40.0mg/L.

Mean measured test concentrations: <0.0067, 1.9, 3.8, 8.4, 16.0, and 33.0/L.

Units-ppm
Value-LC50=12.0 ppm

Test substance : Diethyl phthalate (CAS# 84-66-2)

(1,2,-benzenedicarboxylic acid, diethyl ester)
Synonym: DEP

Conclusion : Test substance is toxic to fish below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document 1.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

08.10.2001 (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : yes
EC50 : m = 86 -
Method : other
Year : 1983
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Method : Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975 Statistical methods-Moving average angle, Probit or Bionomial Concentration.

Result : Analytical samples taken at time zero and on a composite of replicates at termination. Measured values remained consistent during study exposure.

LC50 of 90.0 ppm (based upon Day 0 samples) was recalculated to 86.0 ppm based upon USEPA current practices of using mean of measured initiation and termination samples.1

Nominal test concentrations: control, 50, 86, 140, 240, 400 mg/L.

Measured test concentrations: <0.007, 43, 74, 120, 190, 350 mg/L (Day 0).

Measured concentrations: <0.007, 32, 64, 110, 200, 320 mg/L (Day 2).

Test condition : Test treatments were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 30 minutes. The stock solution was prepared at the highest treatment concentration. Dilutions of the stock were prepared for each treatment level. Three replicates of five organisms were tested per treatment. Test vessels were 250ml beakers with 200ml of test solution. Analytical method was Gas Liquid Chromatography (GLC).

Test temperature=22 +/- 2 Deg C.,
The pH was 8.5 at initiation and ranged from 8.2 to 8.3 at Day 2. Dissolved Oxygen ranged from 7.9 to 8.3 at initiation and 7.9 to 8.4 at Day 2.
Daphnia were <24 hours old and obtained from in-house stock.
Concentrations-Nominal test concentrations: control, 50, 86, 140, 240, 400 mg/L.
Measured test concentrations <0.007, 43, 74, 120, 190, 350 mg/L (Day 0)
Measured concentrations <0.007, 32, 64, 110, 200, 320 mg/L (Day 2).

Test substance : Diethyl phthalate (CAS# 84-66-2)
(1,2,-benzenedicarboxylic acid, diethyl ester)
Synonym: DEP

Conclusion : Test substance is toxic to Daphnia below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference

		document.1
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

08.10.2001 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	
Exposure period	:	8 day
Unit	:	mg/l
Analytical monitoring	:	yes
EC50	:	m = 16 -
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-EPA 600/9-78-018, Printz Algal Assay Bottle Test, 1978. Test type-Static Acute Statistical method-Moving average angle, Probit or Bionomial
Result	:	Value recalculated as 16.0 ppm as per USEPA current practices using mean of measured initiation and termination samples 1. Lowest concentration showed stimulatory effect as compared to the control. In-vivo chlorophyll a, measured daily until less than 5% change. Both cell numbers and in-vivo chlorophyll a, measured at termination. Analytical samples taken at time zero and on a composite of replicates at termination.
Test condition	:	Test substance was added to Algal Growth Medium equal to the highest test concentration (1000ppm) and stirred for one hour and settled for one-half hour. Fifty percent (50%) dilutions were made of this stock solution using algal growth media (dilution water and control) and tested. Initial algal concentration was 2.0x104 cells/ml. Lighting =4,030lux, test temperature=24+/-1 Deg C. The pH range was 7.6 at initiation and 7.9 - 8.9 at day 8. Algal culture stock obtained from Univ. of Texas at Austi Concentrations-Nominal test concentrations: 63, 12.5, 25, 50, 100 ppm. Measured test concentrations = 6.9, 14.5, 28.1, 58.7, 117.5 ppm (Day 0), Measured test concentration = to 0.4, 0.3, 2.3, 1.9 and ND ppm Units-mg/L Value-EC50=30.3 ppm (95% CI of 21.6 - 38.3) based upon Day 0 measured values only.
Test substance	:	Diethyl phthalate (CAS# 84-66-2) (1,2,-benzenedicarboxylic acid, diethyl ester) Synonym: DEP
Conclusion	:	Test substance is toxic to algae at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference documnet.1
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

09.10.2001 (5)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Species	:	rat
Strain	:	
Sex	:	no data
Number of animals	:	3
Vehicle	:	other: Undiluted test material administred
Exposure time	:	6 hour(s)
Value	:	> 4.64 - mg/l
Method	:	other
Year	:	1968
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	There were no death in any animal tested. The ears, nose and paws were red (day post-exposure not specified). All animals gained weight.
Test condition	:	1,2-benzenedicarboxylic acid, diethyl ester (diethyl phthalate) CAS # 84-66-2
Test substance	:	Three rats were exposed for 6 hours to a nominal concentration of 4.64 mg/L of the test substance in a whole-body inhalation chamber. The test substance was heated to 150oC to generate the test atmosphere which was likely a mixture of aerosol and heated vapor. The animals were observed for a period of 14 days for survival.
Conclusion	:	Under the conditions of this study, diethyl phthalate has a low order of acute inhalation toxicity in rats
Reliability	:	(2) valid with restrictions Reliable with restrictions. Screening study; insufficient number of animals. No analytical chamber concentrations or individual animal observations
Flag	:	Critical study for SIDS endpoint

09.10.2001 (11)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Species	:	guinea pig
Strain	:	
Sex	:	no data
Number of animals	:	1
Vehicle	:	other: Undiluted test material administered
Value	:	> 20 - ml/kg bw
Method	:	other
Year	:	1968
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	No animals died. Minimal irritation was observed but not scored. There were no remarkable clinical signs noted during the post-treatment observation period.
Test condition	:	Three guinea pigs were shaved and depilated prior to dosing. Dose levels of 5, 10, or 20 ml/kg of the neat test substance were applied to the skin (one animal per dose level) and the area wrapped with an impervious material for 24 hours. Following unwrapping, the skin was evaluated for signs of irritation. The animals were observed for a period of 14 days for survival.
Test substance	:	1,2-benzenedicarboxylic acid, diethyl ester (diethyl phthalate) CAS # 84-66-2
Conclusion	:	Under the conditions of this study, diethyl phthalate has a low order of

acute dermal toxicity in rats.

Reliability : (2) valid with restrictions
Reliable with restrictions. Screening study; insufficient number of animals.

Flag : Critical study for SIDS endpoint
31.10.2000 (10)

5.4 REPEATED DOSE TOXICITY

Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : oral feed
Exposure period : 16 weeks
Frequency of treatment : Daily for 16 weeks
Post obs. period : Not applicable
Doses : 0 (control), 0.2, 1.0 or 5.0%
Control group : yes, concurrent no treatment
NOAEL : = 150 - 750 mg/kg
Method : other: No data
Year : 1978
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Method : Statistics: Mean values compared to controls by Student's t-test and ranking method of Wilcoxon.
Remark : Short term feeding study: There was a statistically significant decrease in body weights of males and females at 5% and in females only at 1% DEP. Similarly, mean food consumption was decreased in males and females at the high dose and in females at the mid dose. Erythrocyte count was higher in males in the 5% DEP group for 6 weeks compared to controls. This increase was followed by hemoglobin levels that were higher than controls. No significant increases in urinary cell excretion were observed in males or females. The relative weights of the brain, liver, stomach and small intestine were higher in males and females at the high dose compared to controls. The only gross abnormality found during autopsy was a unilaterally small testis in one rat which received DEP (0.2%) in the diet.
Result : NOAEL: males (1% ~ 750 mg/kg/day); females (0.2 %, ~ 150 mg/kg/day).
Test condition : Short term feeding study: Groups of 15 males and females were administered diets containing the doses specified above for 16 weeks. Body weight, food and water intake were measured weekly. At the end of the feeding period, rats were fasted overnight and killed by exsanguination from the aorta. Sections of the following organs were removed and preserved in 10% buffered formalin: brain, pituitary, thyroid, heart, liver, kidney, adrenal glands, spleen, gonads, stomach, small intestine, salivary glands, trachea, lung, thymus, urinary bladder, colon, rectum pancreas, uterus, seminal vesicles, and skeletal muscle. Clinical analyses were performed on blood and urine collected at the post-mortem examination.

Paired-feeding study: Groups of six rats of each sex were fed diets containing either control or 5% DEP for 112 days. Each control was from the same litter as one of the treated rats of the same sex. Food consumption and body weight were recorded daily. Each control rat was given an amount of food equal to that consumed in the previous 24-hour period by its paired littermate. Body weights were measured weekly.
Test substance : 1,2-benzenedicarboxylic acid, diethyl ester (diethyl phthalate)
CAS # 84-66-2
Conclusion : Limited signs of toxicity were observed in male and female rats administered DEP in the diet for periods up to 16 weeks.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
09.10.2001 (7)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium /TA98; TA100; TA1535; TA1537
Concentration : 5 Dose levels up to 10 mg/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year : 1985
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Method : Statistical Methods: A mutagenic response was defined as a reproducible, dose-related increase in the number of histidine-independent colonies over the spontaneous incidence. There was no requirement for a specific magnitude of increase.
Result : The test substance was negative in all strains.
Test condition : Approximately 10E8 bacteria were mixed with 0.5 ml of either 0.1M sodium phosphate buffer or S-9 mix, and test substance. The reaction was carried out in triplicate. The mixture was incubated at 37°C for 48 hours, after which time histidine-revertant colonies were counted. The doses selected were separated by half-log intervals. The high dose was 10 mg/plate unless limited by solubility. Positive control chemicals were sodium azide, nitro-o-phenylenediamine, 9-aminoacridine and 2-aminoanthracene. Concurrent solvent and positive controls were included in all experiments. A toxicity pretest with TA 100 was conducted to determine the high dose level.
Test substance : 1,2-benzenedicarboxylic acid, diethyl ester (diethyl phthalate)
CAS# 84-66-2
Conclusion : No mutagenic activity was observed at doses up to 10 mg/plate in Salmonella strains TA 98, TA 100, TA 1535 and TA 1537 with or without metabolic activation.
Reliability : (1) valid without restriction
1 - Valid without restrictions. NTP-sponsored study.
Flag : Critical study for SIDS endpoint
01.11.2000 (9)

Type : Chromosomal aberration test
System of testing : Non-bacterial: Chinese hamster ovary cells
Concentration : 12.5 hr incubation; 70, 151, and 324 mg/ml
15.5 hr incubation: 70, 151, and 324 mg/ml

Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 473 "Genetic Toxicology: In vitro Mammalian Cytogenetic Test"
Year : 1987
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Method : Statistical tests were performed on both the dose response curve and individual dose points. A statistically significant ($P < 0.05$) difference for one dose point and a significant trend ($P < 0.015$) were considered weak evidence of a positive response; significant differences for two or more doses indicate the trial is positive.

		Metabolic Activation: With and without S9 (metabolic activation enzymes and cofactors from Aroclor 1254-induced male Sprague-Dawley rats)
Result	:	Negative. A small dose-related increase in the percentage of aberrations was observed in one trial without S9; however, this finding was insufficient to be considered positive because no single dose was significantly elevated above the control.
Test condition	:	In the assay without S9, cells were incubated in McCoys 5A medium for 8.5 hours. Colcemid was added and incubation continued for 2 hours. Cells treated with S9 were treated with dimethyl phthalate for 2 hours, after which the treatment medium was removed and cells were then incubated for 10 hours in fresh medium. Colcemid was added during the final 2 hours of the incubation. Cells were selected for scoring based on good morphology and karyotype. Slides were scored blind and were read by the same person. DMSO was used as the solvent control at both incubation time points. Mitomycin-C was used as the positive control at 15.5 hours and cyclophosphamide served as the positive control for the 12.5 hour time point.
Test substance	:	1,2-benzenedicarboxylic acid, diethyl ester (diethyl phthalate) CAS # 84-66-2
Conclusion	:	Under conditions of this study, diethyl phthalate was inactive in the chromosome aberration assay.
Reliability	:	(1) valid without restriction 1 - Valid without restrictions.
Flag	:	Critical study for SIDS endpoint

01.11.2000 (15)

5.8 TOXICITY TO REPRODUCTION

Type	:	Two generation study
Species	:	mouse
Sex	:	male/female
Strain	:	other: Swiss CD-1
Route of admin.	:	oral feed
Exposure period	:	Continuous throughout study (beginning 7 days prior to mating).
Frequency of treatment	:	Daily throughout premating, mating, gestation, and lactation
Premating exposure period		
Male	:	7 days
Female	:	7 days
Duration of test	:	2 generations
Doses	:	0.0, 0.25, 1.25, or 2.5% (~0, 325, 1625, or 3250 mg/kg).
Control group	:	yes, concurrent no treatment
NOAEL Parental	:	= 3250 - mg/kg bw
NOAEL F1 Offspr.	:	= 3250 - mg/kg bw
NOAEL F2 Offspr.	:	= 3250 - mg/kg bw
Method	:	other: continuous breeding study
Year	:	1987
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Statistical methods: Cochran-Armitage (dose-related trends); Fisher's exact test (mating and fertility trends); Kruskal-Wallis test and Jonckheere's test (group means for sex ratio); Wilcoxon-Mann-Whitney U test (pairwise comparisons of treatment group means).
Result	:	NOAEL: 2.5% for fertility and reproductive endpoints. DEP had no effect on the numbers of fertile pairs, the number of litters per pair, the number of pups per litter, live pup birth weight or the proportion of

pups born alive. In the F1 generation, comparisons were made between 0.0 (control) and 2.5% (high dose) animals only. DEP had no effect on fertility, proportion of live births, pup weight or sex. The number of live pups per litter was decreased, however at 2.5%. In addition, statistically significant decreases in body weight were observed in males and females. There were increases male prostate and female liver weight and a decrease in female pituitary weight. DEP had no effect on sperm motility; however, sperm concentration decreased in the treated animals.

Test condition : There were 40 animals/sex in the untreated control group. Males and females in the treatment groups (20 animals/sex) were exposed to the test substance beginning with a 7-day premating period and throughout a cohabitation period for approximately 14 weeks. Reproductive function was assessed during this cohabitation period for number of litters per pair, number of live pups, sex, live births, and pup weight. These litters were subsequently discarded. Following the 14-week cohabitation, the pairs were separated during which any final litters were delivered and kept for assessment of the next generation fertility (F1). When the F1 litters were sexually mature, they were mated with animals from different litters within the same group. The F2 litters were examined for litter size, survival, sex and pup weight. The F1 animals were then necropsied. F0 parameters evaluated: clinical signs, mortality, body weight gain, consumption of food and water. F1 parameters evaluated: reproductive performance, litter size, survival, sex and pup weight F2 parameters evaluated: litter size, survival, sex and pup weight. Sperm examination: Epididymis from the right cauda was excised. The percentage of motile sperm under 400 magnification was determined. Necropsies: In females, endpoints examined included organ weights and histology. In males, organ weights, histology, percentage of motile sperm, sperm concentration and percentage of abnormal sperm was assessed. Clinical observations were performed on blood and urine collected at the post-mortem examination.

Test substance : 1,2-benzenedicarboxylic acid, diethyl ester (diethyl phthalate)
CAS#: 84-66-2

Conclusion : DEP caused decreased body weight gain at 2.5%, but did not affect reproduction. The data from this study confirmed that DEP is not a reproductive toxicant.

Reliability : (2) valid with restrictions
2 - Reliable with restrictions. Only high dose tested in F1 generation.

Flag : Critical study for SIDS endpoint

18.06.2001 (1)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : oral feed
Exposure period : Gestation day 6-15
Frequency of treatment :
Duration of test :
Doses : 0.0, 0.25, 2.5 or 5.0%
Control group : yes
NOAEL Maternalt. : = 1910 - mg/kg bw
NOAEL Teratogen : = 3210 - mg/kg bw
Method : OECD Guide-line 414 "Teratogenicity"
Year : 1993
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Method : Statistical methods: ANOVA; Williams' and Dunnett's Multiple Comparison Test, Fisher's exact probability test.

Result : NOAEL for maternal toxicity: 2.5% (1.91 g/kg/day).
NOAEL for developmental toxicity: 5.0% (3.21 g/kg/day).

Maternal effects: Actual doses received: 0.20, 1.91 and 3.21 g/kg/day based on body weights and food consumption. No dams died during gestation. Food consumption and body weight decreases were observed in the 2.5% and 5.0% treatment groups, however the effect at 2.5% was transient and considered related to the unpalatability of the test feed mix. No effects on kidney or liver weight were observed.

Embryo/fetal effects: No significant findings for number of resorptions, number of implantations, pre- and post-implantation loss or number of corpea lutea. No effects on viability, litter size or mean fetal body weight. No increases in the incidence of fetuses malformed per litter or the percentage of litters with malformations were observed. A statistically significant increased incidence of fetuses exhibiting skeletal variations (particularly supernumerary ribs) was observed at 5.0%, however there was also a high incidence of skeletal variations in the control group. This skeletal variation is generally considered a secondary effect of maternal toxicity and stress, therefore it's significance is unclear.

Test condition : After a 7 day quarantine period, breeding pairs were cohabited overnight. Gestation day 0 was determined the morning that vaginal sperm was found. Initial body weights of females were between 207-273 grams. On gestation day 0, animals were randomly assigned to treatment groups consisting of 25-32 animals. Animals were weighed on the morning of gestation day 0, 3, 6, 9, 12, 15, 18 and 20. In addition, animals were observed daily for signs of toxicity. Maternal body, liver, kidneys, and intact uterus were weighed. Fetuses were weighed, examined for external abnormalities and received a visceral examination.

Test substance : 1,2-benzenedicarboxylic acid, diethyl ester (diethyl phthalate)
CAS # 84-66-2

Conclusion : Under the conditions of this study, DEP was not a selective developmental toxicant. DEP exposure was associated with maternal effects and an increased incidence in fetal supernumerary ribs at the highest dose tested (5.0%).

Reliability : (1) valid without restriction
1 - Valid without restrictions; guideline study.

Flag : Critical study for SIDS endpoint

18.06.2001 (12)

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : i.p.
Exposure period : Gestation days 5, 10 and 15
Frequency of treatment :
Duration of test : Gestation day 20
Doses : 0.51, 1.01, and 1.68 ml/kg (~560, 1100, and 1880 mg/kg)
Control group : yes
Method : other
Year : 1972
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Method : Statistical methods: Students t-test; Methods of Weil (1952) and Cornfield and Mantel (1950).

Result : Maternal Effects: Limited information on maternal effects (food consumption, body weight changes, deaths) were provided.

Embryo/fetal effects: Skeletal abnormalities were observed with all three dose levels of diethyl ester. These observations included elongated and fused ribs, incomplete skull bones, incomplete or missing leg bones. No

evidence of gross malformations or dead fetuses were recorded following administration of diethyl phthalate. Resorptions were found at the low dose of diethyl ester (3.6%) and at the high dose (44.4%).

Test condition : Female rats were selected after observation of at least two complete estrous cycles. The onset of gestation was determined by the presence of sperm in the vaginal smear. The onset of gestation was recorded as Day 0. Diethyl ester was administered to rats at doses representing one-tenth, one-fifth, and one-third of the acute LD50. On the day before parturition (day 20), each rat was sacrificed by an overdose of ether. Following sacrifice, the numbers of corpora lutea, resorption sites and viable and dead fetuses were recorded. Fetuses were also examined for skeletal malformation and variations.

Test substance : 1,2-benzenedicarboxylic acid, diethyl ester (diethyl phthalate)
CAS # 84-66-2

Conclusion : Although fetal data were provided, it is difficult to place these data into the proper context without information regarding toxic effects to the dams. Also, conventional developmental toxicity study designed was not used in this study.

Reliability : (3) invalid
3 - Not reliable. Non-standard study design; insufficient data.

01.11.2000 (2)

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1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

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7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the Low Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There is a large amount of data for the physicochemical properties of dimethyl and diethyl phthalate. Computer models were also used to estimate these properties for comparison with measured values and additionally were used to predict environmental distribution.

A complete health effects SIDS data set is available for diethyl phthalate, and for dimethyl phthalate with the exception of adequate reproductive data. Both DMP and DEP show minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for developmental effects. Although adequate reproductive data are not available for DMP, data on DEP indicate that this material will not cause reproductive effects. This is further supported by data showing that neither DEP nor DMP had effects on male reproductive development. The lack of developmental effects observed with DMP, coupled with chronic toxicity studies showing no effects on reproductive organs, negates the need to conduct a reproductive study for DMP.

There are numerous published acute aquatic toxicity studies in a variety of species of fish, daphnia and algae for DMP and DEP. DMP and DEP are slightly soluble in aqueous systems. Acute effects on aquatic species are seen in the 10 to 100 ppm range.

02.11.2001

7.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 27554-26-3
CAS No.	:	27554-26-3
EINECS Name	:	diisooctyl phthalate
EINECS No.	:	248-523-5
TSCA Name	:	1,2-Benzenedicarboxylic acid, diisooctyl ester
Molecular Formula	:	C24H38O4

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	01.11.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	01.11.2000
Memo	:	ACC Phthalate Esters Panel HPV Task Group
Printing date	:	05.11.2001
Revision date	:	
Date of last Update	:	10.10.2001
Number of Pages	:	15
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers:68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6, and 111381-90-9.

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from

alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate categories. Of the phthalates in this category, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

05.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

2.1 MELTING POINT

Value	:	-46 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	
Remark	:	Literature review collecting data from a variety of sources. Manufacturer's data or handbook value
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(4) not assignable

10.10.2001 (9)

Value	:	64 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation Melting point calculation seems to give erroneously high results for the phthalate esters
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(3) invalid

10.10.2001 (8)

2.2 BOILING POINT

Value	:	417 - ° C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	
GLP	:	
Test substance	:	
Method	:	Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (8)

Value	:	>300 ° C at 1013 hPa
Decomposition	:	no
Method	:	other (measured)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Manufacturer's data or handbook value.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(4) not assignable

10.10.2001 (11)

2.4 VAPOUR PRESSURE

Value : .000000249 - hPa at 25° C
Decomposition : no
Method other (measured)
Year : 2000
GLP :
Test substance :
Decomposition : no
Remark : Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (1) valid without restriction
15.12.2000 (4)

Value : .00000133 - hPa at 25° C
Decomposition : no
Method other (measured)
Year : 2000
GLP :
Test substance :
Decomposition : no
Remark : Literature review collecting data from a variety of sources.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (9)

Value : .00000185 - hPa at 25° C
Decomposition : no
Method other (calculated)
Year : 2000
GLP :
Test substance :
Decomposition : no
Method : Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001 (8)

2.5 PARTITION COEFFICIENT

Log pow : 7.73 - at 25° C
Method other (measured)
Year : 2000
GLP :
Test substance :
Remark : Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (1) valid without restriction
15.12.2000 (4)

Log pow	:	8.39 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (8)

2.6.1 WATER SOLUBILITY

Value	:	.00024 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (8)

Value	:	.00249 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

15.12.2000 (4)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.00000000002056 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (8)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	3.4 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	
Method	:	
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (8)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.027
Water (level I)	:	.0005
Soil (level I)	:	97.7
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (7)

3.3.2 DISTRIBUTION

Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level I
Year	:	2000
Result	:	Soil - 97.7% Air - 0.0027% Water - 0.00045% Sediment - 2.17% Suspended sed. - 0.068%
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (7)

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	domestic sewage
Concentration	:	20mg/l related to Test substance related to
Contact time	:	28 day
Degradation	:	= 57 - % after
Result	:	readily biodegradable
Deg. Product	:	
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA 1982, CO2 Evolution, Shake Flask (modified Gledhill). Inoculum-Domestic sewage, soil, and mineral medium. Kinetics-Not Reported Degradation Products-Not Reported Analytical Monitoring-Yes
Result	:	Primary degradation is expressed as the loss of initial test substance. Ultimate biodegradation is expressed as the percentage of ThCO2 in each flask. Units-% biodegradation Value->99% primary, and 57% ultimate biodegradation.
Test condition	:	Inoculum was aged for 2 weeks prior to test initiation. The test chemical was added to flasks containing medium and inoculum. The flask were incubated and shaken in the dark for 28 days. Three replicates for CO2 evaluation and 4 replicates for primary degradation were tested. The CO2 production was captured in barium hydroxide solution. Primary biodegradation was determined at the beginning, middle and end by GC FID of entire contents of one replicate. A glucose and blank were also tested. 2L Erlenmeyer flasks were used as test vessels. The pH at initiation was 7.0 to 7.2. Test flasks were shaken at a rate of 120rpm at 22 +/- 2 Deg C. Nominal test concentration = 20mg/L for test substance and glucose.
Test substance	:	Diisooctyl Phthalate (CAS# 27554-26-3) (1,2,-benzenedicarboxylic acid, diisooctyl ester) Synonym: DIOP
Conclusion	:	The substance is readily biodegradable using mixed populations of microorganisms,
Reliability	:	(2) valid with restrictions

Flag : Critical study for SIDS endpoint
29.11.2000 (10)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	m > .23 -
Method	:	other
Year	:	1982
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians. Statistical methods-Moving average angle, Probit or Bionomial
Result	:	Mean measured values used in calculation of LC50. Analytical samples taken at time zero and on a composite of replicates at termination. Measured values remained consistent during the exposure period. Fish mean Total length=39mm, mean wet weight=0.5g Value-LC50=>0.23 ppm
Test condition	:	Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15L of solution. The diluter maintained a water turnover rate of 5-8 tank volumes per day. Two replicates of ten organisms were tested per treatment. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection. Test temperature=11 +/- 1 Deg C., The pH range was 7.1 to 7.5. The mean Dissolved Oxygen ranged from 9.5 to 9.6mg/L. Fish were obtained from Montana. Nominal test concentrations: control, 0.018, 0.036, 0.072, 0.14, and 0.29mg/L. Mean measured test concentrations: <0.0040, 0.017, 0.031, 0.060, 0.11, and 0.23mg/L.
Test substance	:	Diisooctyl Phthalate (CAS# 27554-26-3) (1,2,-benzenedicarboxylic acid, diisooctyl ester) Synonym: DIOP
Conclusion	:	Test substance is non-toxic to fish at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document.1
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

29.11.2000 (2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)

Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	m > .22 -
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975 Statistical methods-Moving average angle, Probit or Bionomial
Result	:	Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined slightly during study exposure. More than 50% of the daphnids were trapped at the surface or on air bubbles in all concentrations except the Control. A repeat study was performed at a loading of 10mg/L with a measured value of 0.22ppm. No mortality was observed at this highest water soluble concentration, confirming the first set of results. Value-LC50=>0.22 ppm (based upon second study results).
Test condition	:	Test treatments were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 2 minutes. Dilutions of the stock were prepared for each treatment level. The stock solution was prepared at the highest treatment concentration. Three replicates of five organisms were tested per treatment. Test vessels were 250ml beakers with 200ml of test solution. Analytical method was Gas Liquid Chromatography (GLC). Test temperature=22 +/- 2 Deg C., The pH ranged from 8.3 to 8.5 at initiation and 8.4 to 8.5 at Day 2. Dissolved Oxygen ranged from 8.5 to 9.0 at initiation and 7.6 to 7.9 at Day 2. Daphnia were <24 hours old and obtained from in-house stock. Nominal test concentrations: control, 0.032, 0.055, 0.090, 0.15, and 0.25mg/L. Measured test concentrations <0.0037, 0.024, 0.039, 0.065, 0.11, 0.18(Day 0) Measured concentrations <0.0037, 0060, 0.015, 0.030, 0.068, 0.090 (Day 2),
Test substance	:	Diisooctyl Phthalate (CAS# 27554-26-3) (1,2,-benzenedicarboxylic acid, diisooctyl ester) Synonym: DIOP
Conclusion	:	Test substance is non-toxic to Daphnia at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document.1
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

29.11.2000 (1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	
Exposure period	:	6 day
Unit	:	
Analytical monitoring	:	yes
EC50	:	m > 1.3 -
Method	:	other

Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-EPA 600/9-78-018, Printz Algal Assay Bottle Test, 1978. Test Type-Static Acute Statistical methods-Moving average angle, Probit or Bionomial
Result	:	In-vivo chlorophyll a, measured daily until less than 5% change. Both cell numbers and in-vivo chlorophyll a, measured at termination. Analytical samples taken at time zero and on a composite of replicates at termination. Value-EC50=>2.0 ppm based upon Day 0 measured values only. 1Value recalculated as >1.3 ppm as per USEPA current practices using mean of measured initiation and termination samples.1
Test condition	:	Algal Growth Medium was used as the control and diluent. 10uL of test substance was added to 1.0L of sterile water to form a saturated phthalate solution. This solution was sonicated for 1 minute and allowed to settle for 4 hours. After settling, the water soluble fraction (WSF) was removed for testing. Initial algal concentration was 2.0x104 cells/ml. Only one treatment level was evaluated (100%WSF). Based upon earlier phthalate testing, toxicity was not expected. Lighting =4,500lux, test temperature=22+/-2 Deg C. The pH range was 7.7 at initiation and 7.7 - 7.8 at Day 6. Algal culture stock obtained from Univ. of Texas at Austin. Nominal test concentrations: 100% WSF (10ul/L stock). Measured test concentrations = 2.0 ppm on Day 0, Measured test concentration = 0.6ppm on Day 6
Test substance	:	Diisooctyl Phthalate (CAS# 27554-26-3) (1,2,-benzenedicarboxylic acid, diisooctyl ester) Synonym:DIOP
Conclusion	:	Test substance is not toxic to algae at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document.1
Reliability	:	(2) valid with restrictions Control chlorophyll or cell counts not reported.
Flag	:	Critical study for SIDS endpoint

29.11.2000 (3)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Bacterial
Concentration	:	10- 2000 mg/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year	:	1985
GLP	:	no
Test substance	:	other TS
Test substance	:	1,2,-benzenedicarboxylic acid, diisooctyl ester (diisooctyl phthalate)
Conclusion	:	Under conditions of this study, diisooctyl ester was not mutagenic in the Ames mutation assay.
Reliability	:	(4) not assignable

02.01.2001 (6)

6. References

(1) CMA Study, Acute Toxicity of Fourteen Esters to Daphnia magna., Springborn Bionomics, Inc. 1984. Report # BW-84-4-1567.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(2) CMA Study, Acute Toxicity of Fourteen Esters to Rainbow Trout Salmo gairdneri Under Flow-Through Conditions. EG&G Bionomics, Inc. 1983. Report # BW-83-3-1373, Performed Jul 1982 to Jan 1983.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(3) CMA Study, Toxicity of Fourteen Esters to the Freshwater Green Alga Selenastrum capricornutum. 1984, Springborn Bionomics, Inc. Performed 4-10 Nov 1983.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(4) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, Chemosphere 41:1389-1399.

(6) Goodyear Fiber and Polymer Products Research Division Laboratory. Mutagenicity evaluation of diisooctyl phthalate (USS Chemical). Report No 81-4-7; EPA Document 878210369.

(7) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(8) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(9) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997), the Environmental Fate of Phthalate Esters: A literature Review, Chemosphere 35:667-749.

(10) Sugatt, R.H. et al, 1983 Shake Flask Biodegradation of 14 Commercial Phthalate Esters. Syracuse Research Corporation, Syracuse, NY. SRC# L1543-05. Performed for CMA.

(11) David, R., R. McKee, J. Butala, R. Barter and M. Kayser (2001), Chapter 80 - Esters of Aromatic Mono, Di and Tricarboxylic acids and Di, Tri, or Polyalcohols, Patty's Toxicology, 5th edition, Vol 6., J Wiley & Sons, Inc. pp 635-932.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2, 3, 4 & 5

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 84-75-3
CAS No.	:	84-75-3
EINECS Name	:	Dihexyl phthalate
Molecular Weight	:	334.5
Molecular Formula	:	C20H30-O4

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.11.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.11.2000
Memo	:	ACC Phthalate Esters Panel HPV Testing group
Printing date	:	05.11.2001
Revision date	:	
Date of last Update	:	05.11.2001
Number of Pages	:	13
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers:68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6, and 111381-90-9.

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from

alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate categories. Of the phthalates in this category, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

05.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

2.1 MELTING POINT

Value	:	48 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	
Remark	:	Literature review collecting data from a variety of sources. Manufacturer's data or handbood value.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

09.10.2001 (10)

2.2 BOILING POINT

Value	:	385 ° C at 1013 hPa
Decomposition	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	
Method	:	Boiling point calculation by MPBPWIN ver 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

09.10.2001 (10)

2.4 VAPOUR PRESSURE

Value	:	= .00000345 - hPa at ° C
Decomposition	:	
Method		other (calculated)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

05.11.2001 (3)

Value	:	= .0000161 - hPa at ° C
Decomposition	:	
Method		other (calculated)
Year	:	
GLP	:	
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

Reliability : (2) valid with restrictions
05.11.2001

(10)

2.5 PARTITION COEFFICIENT

Log pow : = 6 - at ° C
Method other (measured)
Year :
GLP :
Test substance :
Remark : Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (1) valid without restriction
09.10.2001

(2)

Log pow : = 6.5 - at ° C
Method other (calculated)
Year :
GLP :
Test substance :
Method : Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark : EPIWIN is used and advocated by the US EPA for chemical proterty estimation.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
09.10.2001

(10)

2.6.1 WATER SOLUBILITY

Value : = - .0115 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other: calculated
Year : 2000
GLP :
Test substance :
Method : Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard EPIWIN is used and advocated by the US EPA for chemical property estimation.
Source : ExxonMobil Biomedical Science, Inc. Annandale, N.J. USA
Reliability : (1) valid without restriction
05.11.2001

Value : = - .159 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other
Year :
GLP :
Test substance :
Remark : Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (1) valid without restriction
05.11.2001

(10)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	- based on Intensity of Sunlight
Indirect photolysis		
Sensitizer	:	
Conc. of sens.	:	
Rate constant	:	= .00000000001493 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

09.10.2001 (10)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	= 3.4 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on workd for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

05.11.2001 (10)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	
Media	:	
Air (level I)	:	.28
Water (level I)	:	.03
Soil (level I)	:	97.5
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

09.10.2001 (8)

3.3.2 DISTRIBUTION

Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level I
Year	:	
Result	:	Soil - 97.5% Air - 0.28% Water - 0.03% Sediment - 2.17%
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

09.10.2001 (8)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	male/female
Number of animals	:	
Vehicle	:	no data
Value	:	= - 29.6 ml/kg bw
Method	:	other
Year	:	1973
GLP	:	no
Test substance	:	other TS
Result	:	LD50 = 29.6 ml/kg (males); 38.9 ml/kg (females).
Test substance	:	1,2-benzenedicarboxylic acid, dihexyl ester (di-n-hexyl phthalate)
Conclusion	:	The acute oral LD50 was reported as 29.6 ml/kg (males) and 38.9 ml/kg (females).
Reliability	:	(4) not assignable No experimental detail presented; LD50 values reported from unpublished sources.

15.12.2000 (6)

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male
Strain	:	Wistar
Route of admin.	:	oral feed
Exposure period	:	21 Days
Frequency of treatment	:	Daily
Post obs. period	:	None
Doses	:	0, 2.0% (20 g/kg in diet, estimated 1800 mg/kg/day).
Control group	:	yes
Method	:	
Year	:	1985
GLP	:	no data
Test substance	:	other TS
Remark	:	There was no effect on food consumption or body weight gain. Liver weights were statistically increased at the terminal sacrifice (21 days). Light microscopy of the livers of the treated animals after 10 and 21 days revealed centrilobular accumulation of fat associated with some necrosis. Examination via electron microscopy showed accumulation of small lipid droplets in hepatocytes after 10 days and progression to larger droplets after 21 days. There was also some evidence of a small increase in peroxisome number. There were no biologically significant changes in liver enzymes or other biochemical analyses.
Result	:	NOAEL not determined.
Test condition	:	Following a one week acclimation period, the test or control diets were given to the rats for 21 days. The animals were observed daily and food consumption measured twice weekly. Subgroups of 4 rats were sacrificed at 3, 10 and 21 days. Liver, testes, epididymis, and seminal vesicles were weighed. Liver, kidneys, spleen, testes, epididymis, and seminal vesicles were preserved for microscopic examination. A portion of the liver also was used for enzyme and biochemical determinations
Test substance	:	1,2-benzenedicarboxylic acid, dihexyl ester (di-n-hexyl phthalate)
Conclusion	:	Diets containing a high concentration of DnHP induced accumulation of

large droplets of fat in liver centrilobular regions with mild necrosis. There were increased liver weights and evidence of a slight induction of peroxisomes, but no significant changes in any other parameters.

Reliability : (2) valid with restrictions
Screening study with single dose level an limited number of animals.

19.06.2001 (9)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Bacterial
Concentration	:	5 dose levels up to 10 mg/plate.
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year	:	1985
GLP	:	no data
Test substance	:	other TS
Method	:	Statistical Methods: A mutagenic response was defined as a reproducible, dose-related increase in the number of histidine-independent colonies over the spontaneous incidence. There was no requirement for a specific magnitude of increase.
Result	:	The test substance was negative in all strains.
Test condition	:	Approximately 10E8 bacteria were mixed with 0.5 ml of either 0.1M sodium phosphate buffer or S-9 mix, and test substance. The reaction was carried out in triplicate. The mixture was incubated at 37°C for 48 hours, after which time histidine-revertant colonies were counted. The doses selected were separated by half-log intervals. The high dose was 10 mg/plate unless limited by solubility. Positive control chemicals were sodium azide, nitro-o-phenylenediamine, 9-aminoacridine and 2-aminoanthracene. Concurrent solvent and positive controls were included in all experiments. A toxicity pretest was conducted to determine the high dose level. This study was conducted with TA 100 in the presence and absence of S-9.
Test substance	:	1,2-benzenedicarboxylic acid, dihexyl ester (di-n-hexyl phthalate)
Conclusion	:	No mutagenic activity was observed at doses up to 10 mg/plate in Salmonella strains TA 98, TA 100, TA 1535 and TA 1537 with or without metabolic activation.
Reliability	:	(1) valid without restriction

19.06.2001 (5)

5.8 TOXICITY TO REPRODUCTION

Type	:	Two generation study
Species	:	mouse
Sex	:	male/female
Strain	:	CD-1
Route of admin.	:	oral feed
Exposure period	:	Continuous throughout study (beginning 7 days prior to mating).
Frequency of treatment	:	Daily throughout premating, mating, gestation, and lactation.
Premating exposure period		
Male	:	7 Days (continuous)
Female	:	7 Days (continuous)
Duration of test	:	2 generations

Doses	:	0.0, 0.3, 0.6, or 1.2% (0, 430, 880, and 1870 mg/kg/day)
Control group	:	yes
Method	:	other
Year	:	1987
GLP	:	no data
Test substance	:	other TS
Method	:	Control Group: 40 males and 40 females. Statistical Methods: Cochran-Armitage (dose-related trends); Fisher's exact test (mating and fertility trends); Kruskal-Wallis test and Jonckheere's test (group means for sex ratio); Wilcoxon-Mann-Whitney U test (pairwise comparisons of treatment group means).
Remark	:	Exposure to DnHP did not affect food consumption but did produce a dose-related decrease in body weight after 13 weeks. There were no litters in the 1.2% group and only 1 pair produced a litter in the 0.6% group compared to all 37 pairs delivering at least one litter in the control group and 14 of 17 pairs in the 0.3% group. The 0.3% group exhibited reduced number of litters per pair, number of live pups/litter, and proportion of live pups. The crossover mating study revealed reduced fertility in both sexes - only 1 of 18 high-dose males sired a litter and none of the high-dose females became pregnant. Sperm assessment of the high-dose males showed that the % motile sperm and sperm concentration were decreased, although the % abnormal sperm was not increased. There were significant decreases in weights of testes, epididymis, and seminal vesicles; atrophy of the seminiferous tubules was observed microscopically. There were no apparent changes in the female high-dose reproductive organs. Kidney and adrenal weights were decreased, and liver weights increased in both sexes at the high dose although no histopathologic changes were found.
Result	:	NOAEL - not determined. LOAEL - 0.3% (430 mg/kg/day) for fertility and reproductive endpoints.
Test condition	:	There were 40 animals/sex in the untreated control group. Males and females in the treatment groups (20 animals/sex) were exposed to the test substance beginning with a 7-day premating period and throughout a cohabitation period for approximately 14 weeks. Reproductive function was assessed during this cohabitation period for number of litters per pair, number of live pups, sex, live births, and pup weight. These litters were subsequently discarded. Following the 14-week cohabitation, the F0 pairs were separated but continued treatment. Any final litters that were delivered during this time were kept for at least 21 days (weaning). The F0 males and females were necropsied, organs weighed and microscopically examined. Sperm assessment also was performed for the males. A crossover mating trial was then performed to determine whether F0 males or females were more sensitive to adverse effects. High-dose mice of each sex were mated to control mice and the offspring of these crossover matings were examined for litter size, sex, and pup weight. The parents were necropsied.
Test substance	:	1,2-benzenedicarboxylic acid, dihexyl ester (di-n-hexyl phthalate)

15.12.2000 (7)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	mouse
Sex	:	female
Strain	:	CD-1
Route of admin.	:	gavage
Exposure period	:	Gestation days 6-13
Frequency of treatment	:	Daily
Duration of test	:	7 days
Doses	:	10 ml/kg/day (9900 mg/kg/day)

Control group	:	yes, concurrent vehicle
Method	:	other
Year	:	1987
GLP	:	no data
Test substance	:	other TS
Method	:	Control Group: 50 females; corn oil only. Statistical Methods: ANOVA (maternal body weights at gd6); Fischer's exact test (mortality and number of viable litters); Mann Whitney U-test (maternal body weight gd6 to pd3, number live births, pup survival, pup weight and weight gain).
Result	:	NOAEL: Not determined. Maternal Effects: One mouse died during the study (1/48). No other maternal effects were reported. Embryo/fetal effects: There were no viable litters from 34 confirmed-mated females.
Test condition	:	Fifty timed-pregnant female mice were dosed daily on gestation days 6-13 with the test substance. A single dose level of 10 ml/kg was used as the highest practical level due to lack of toxicity (LD10 could not be established). Litters were held until postpartum day 3 then discarded. The following data were recorded: maternal observations, survival, and weight gain from gestation day 6 to postpartum day 3; number of live births, number of viable litters, total litter weight, litter weight gain, and pup survival.
Test substance	:	1,2-benzenedicarboxylic acid, dihexyl ester (di-n-hexyl phthalate)
Reliability	:	(2) valid with restrictions Screening study only; non-standard study design with limited data.

19.06.2001 (1)

(1) B. D. Hardin, R. Schuler, J. Burg, G. Booth, K. Hazelden, K. MacKenzie, V. Piccirillo and K. Smith (1987). Evaluation of 60 chemicals in a preliminary developmental toxicity test. Teratogenesis, Carcinogenesis and Mutagenesis 7:29-48 .

(2) Cousins, I. and D. Mackay (2000), Correlating the Physical-Chemical Properties of Phthalate Esters Using the "Three Solubility" approach, Chemosphere 41:1389-1399.

(3) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Esters Usingthe Three Solubility' approach, Chemosphere 41:1389-1399.

(5) E. Zeiger, S. Haworth, K. Mortelmans, and W. Speck (1985). Mutagenicity Testing of Di(2-ethylhexyl) phthalate and Related Chemicals in Salmonella. Environmental Mutagenesis 7: 213-232.

(6) Krauskpf, L. (1973). Studies on the toxicity of phthalates via ingestion. Environmental Health Perspectives 3:61-72.

(7) Lamb, J.C., Chapin, R.E., Teague, J., Lawton, A.D., and Reel, J.R. (1987). Reproductive effects of four phthalic acid esters in the mouse. Toxicology and Applied Pharmacology 88:255-269.

(8) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available from the Enviromental Center, Trent University. Canada.

(9) Mann. A.H., Price, S.C., Mitchell, P.G., Hinton, R.H., and Bridges, J.W. (1985). Comparison of the Short-Term Effects of Di(2-ethylhexyl)Phthalate, Di(n-hexyl)Phthalate, and Di(n-octyl)Phthalate in Rats. Toxicol.. Appl. Pharmacol. 77:116-132.

(10) Meylan, M. Syracuse Research Corporation (1994-1999).
Calculation program contained in EPIWIN (Esitmate Ver. 3.04) available from SRC.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2, 3, 4 & 5

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 68515-44-6
CAS No.	:	68515-44-6
TSCA Name	:	1,2,-benzenedicarboxcylic acid, diheptyl ester, branched and linear
Generic name	:	diheptyl phthalate, branched and linear
Synonym	:	Phthalic acid, dialkyl(C7) ester

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - transitional phthalates
Printing date	:	05.11.2001
Revision date	:	
Date of last Update	:	05.11.2001
Number of Pages	:	12
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers:68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6, and 111381-90-9.

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from

alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate categories. Of the phthalates in this category, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

05.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

2.1 MELTING POINT

Value : -45 - ° C
Decomposition : no at - ° C
Sublimation : no
Method :
Year :
GLP :
Test substance :
Remark : Literature review collecting data from a variety of sources.
Manufacturer's data or handbook value
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
14.12.2000 (7)

Value : 43 - ° C
Decomposition : no at - ° C
Sublimation : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Melting point calculation by MPBBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Melting point calculation seems to give erroneously high results for the phthalate esters
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (3) invalid
10.10.2001 (6)

2.2 BOILING POINT

Value : 364 - ° C at 1013 hPa
Decomposition : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Boiling point calculation by MPBBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001 (6)

Value : >300 ° C at 1013 hPa
Decomposition : no
Method : other
Year : 2000
GLP :
Remark : Manufacturer's data or handbook value.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (4) not assignable
10.10.2001 (2)

2.4 VAPOUR PRESSURE

Value	:	.000000933 - hPa at 25° C
Decomposition	:	no
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Decomposition	:	no
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (1)

Value	:	.0000108 - hPa at 25° C
Decomposition	:	
Method		other (calculated)
Year	:	
GLP	:	
Test substance	:	
Method	:	Vapor pressure calculation by MPBBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (6)

2.5 PARTITION COEFFICIENT

Log pow	:	6.87 - at 25° C
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (1)

Log pow	:	7.41 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (6)

2.6.1 WATER SOLUBILITY

Value	:	.00245 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (6)

Value	:	.02 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.00000000001872 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (6)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	4.2 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

14.12.2000 (6)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.138
Water (level I)	:	.0043
Soil (level I)	:	97.6
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

Reliability : (2) valid with restrictions
14.12.2000 (5)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year :
Result : Soil - 97.6%
Air - 0.138%
Water - 0.00429%
Sediment - 2.169%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
14.12.2000 (5)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Mouse lymphoma assay
System of testing	:	Mammalian Cell
Concentration	:	0.125 to 6 ul/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year	:	2000
GLP	:	yes
Test substance	:	other TS: 711P
Method	:	Statistical Methods: The minimum criterion necessary to demonstrate mutagenesis was a mutation frequency that was at least 1.5 times the concurrent background frequency plus 10 x 10-6. The background frequency was defined as the average mutant frequency of the solvent negative controls. Control Groups: The negative control article was the solvent (acetone) used in the assay. Ethylmethane sulfonate (EMS) was used as a positive control in the assays without S9 activation. 3-methylcholanthrene which requires metabolic activation, was used as a positive control for assays with S9.
Result	:	Negative In the absence of activation, 0.75 to 6.0 ul/ml induced moderate to high toxicity (percent relative growths: 3.2% to 48.4%), but only a slight increase in mutation frequency at the highest doses. In the presence of a metabolic fraction, 0.125 to 1.5 ul/ml resulted in percent relative growths of 8.9% to 82.2% without increasing the incidence of mutations. Thus, the test compound was considered non-mutagenic in this assay.
Test condition	:	Mouse lymphoma cells were seeded into a series of tubes at 6 x 106 cells per tube. Dosed tubes were exposed for 4 hours to the test substance. An expression period of 48 hours was used; after the 48 hour expression time, 3 x 106 cells per plate were added to semi-solid selection medium containing 3 ug/ml trifluorothymidine (TFT) to score for mutant colonies and 200 cells per plate were added to cloning medium, without TFT, to evaluate viability. Mutant frequencies were calculated after 10-14 days incubation. Mutant and total colony count at each dose level were determined by triplicate plates.
Test substance	:	Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11). Data used as read-across to 1,2-benzenedicarboxylic acid, diheptyl ester (diheptyl phthalate); CAS# 68515-44-6.
Conclusion	:	Under conditions of this study the test substance was non-mutagenic in the mouse lymphoma assay with or without metabolic activation.
Reliability	:	(1) valid without restriction

05.11.2001 (3)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	9 days
Frequency of treatment	:	Daily
Duration of test	:	20 Days
Doses	:	0, 40, 200, 1000 mg/kg/day
Control group	:	yes, concurrent vehicle
NOAEL Maternalt.	:	= 200 - mg/kg bw
NOAEL Teratogen	:	= 200 - mg/kg bw
Method	:	OECD Guide-line 414 "Teratogenicity"
Year	:	2000
GLP	:	yes
Test substance	:	other TS: 711P
Method	:	Control Group: Olive oil vehicle control. Statistical Methods: Dunnett's Test for food consumption, body weight, organ weight, placental and fetal data; Fisher's Exact Test for female mortality, litters with findings; and the Wilcoxon Test for proportion of fetuses with findings per litter.
Result	:	Maternal Effects: There were no treatment-related effects in the 40 or 200 mg/kg/day groups either in the dams or fetuses. The high dose (1000 mg/kg/day) maternal body weights were decreased during gestation days 15-20, and relative liver and kidney weight was increased in the high dose group dams. Six of the ten high dose dams showed vaginal hemorrhage during the study; three had complete resorptions. Embryo/fetal effects: Fetal weights of the remaining viable litters were reduced, and all litters contained malformations. The malformations affected mainly the brain, vertebral column, tail, scapula, sternum, and urogenital tract. In total, 47/53 high-dose fetuses (89%) from all seven litters were malformed.
Test condition	:	Eight to ten pregnant females were used per group. Animals were weighed on gestation days 0, 6, 10, 15, and 20, and observed daily for signs of toxicity. On GD 20, animals were sacrificed and maternal body, liver, kidneys, and intact uterus were weighed. Fetuses were weighed, examined for external and visceral abnormalities.
Test substance	:	Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11). Data used as read-across to 1,2-benzenedicarboxylic acid, diheptyl ester (diheptyl phthalate); CAS# 68515-44-6.
Conclusion	:	Significant maternal and fetal effects only were observed at the high dose (1000 mg/kg/day). No treatment-related effects were observed in the 40 or 200 mg/kg/day groups.
Reliability	:	(2) valid with restrictions

05.11.2001 (4)

6. References

(1) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, Chemosphere 41:1389-1399.

(2) David, R., R. McKee, J. Butala, R. Barter and M. Kayser (2001), Chapter 80 - Esters of Aromatic Mono, Di and Tricarboxylic acids and Di, Tri, or Polyalcohols, Patty's Toxicology, 5th edition, Vol 6., J Wiley & Sons, Inc. pp 635-932.

(3) E. Barber, M. Cifone, J. Rundell, R. Przygoda, B. Astill, E. Moran, A. Mulholland, E. Robinson and B. Schneider. (2000). Results in the L5178Y mouse lymphoma and the in vitro transformation of Balb 3T3 cell assays for eight phthalate esters. Journal of Applied Toxicology 20:69-80.

(4) J. Hellwig, H. Freudenberger and R. Jackh. (1997). Differential prenatal toxicity of branched phthalate esters in rats. Food and Chemical Toxicology 35:501-512.

(5) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(6) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(7) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997), the Environmental Fate of Phthalate Esters: A literature Review, Chemosphere 35:667-749.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2, 3, 4 & 5

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 68515-50-4
CAS No.	:	68515-50-4
TSCA Name	:	1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Generic name	:	dihexyl phthalate, branched and linear

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - transitional phthalates
Printing date	:	05.11.2001
Revision date	:	
Date of last Update	:	10.10.2001
Number of Pages	:	17
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers:68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6, and 111381-90-9.

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from

alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate categories. Of the phthalates in this category, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

05.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

2.1 MELTING POINT

Value	:	-27 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	
Remark	:	Literature review collecting data from a variety of sources. Manufacturer's data or handbook value
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (12)

Value	:	49 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation Melting point calculation seems to give erroneously high results for the phthalate esters
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(3) invalid

09.10.2001 (11)

2.2 BOILING POINT

Value	:	373 - ° C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Reliability	:	(2) valid with restrictions
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

09.10.2001 (11)

Value	:	340 ° C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	2000
GLP	:	
Reliability	:	(4) not assignable
Remark	:	Manufacturer's data or handbook value.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

09.10.2001 (5)

2.4 VAPOUR PRESSURE

Value	:	.00000344 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	
GLP	:	
Test substance	:	
Decomposition	:	no
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (4)

Value	:	.0000301 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

09.10.2001 (11)

2.5 PARTITION COEFFICIENT

Log pow	:	6 - at 25° C
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (4)

Log pow	:	6.46 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (11)

2.6.1 WATER SOLUBILITY

Value	:	.023 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

09.10.2001 (11)

Value	:	.159 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (4)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.00000000001129 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (11)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	3.5 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (11)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.334
Water (level I)	:	.038
Soil (level I)	:	97.4
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

Reliability : (2) valid with restrictions
09.10.2001 (10)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 2000
Result : Soil - 97.4%
Air - .33%
Water - 0.04%
Sediment - 2.16%
Suspended sed. - 0.07%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
09.10.2001 (10)

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge
Concentration : 36.39mg/l related to Test substance
related to
Contact time :
Degradation : = 79.66 - % after 28 day
Result : readily biodegradable
Control substance : other
Kinetic : - %
- %
Deg. Product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year : 1983
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Method : OECD 301F, Raedy Biodegradability, Manometric Respirometry Test. Analytical Monitoring-None
Result : The degradation calculation was performed using the respirometry software and the Theoretical Oxygen Demand (ThOD) and the mass of the test substance added. ThOD based upon the elemental analysis of the test substance.

Test substance biodegradation = 79.66% (sd 10.02)
Positive Control degradation = 94% by Day 14.
Test condition : Treatment replicates were prepared by combining glass-distilled water, a mineral substrate, pH buffer, activated sludge and the appropriate test substance.
Three replicates of the test material and two replicates of positive control (sodium benzoate) were prepared and evaluated in 1L glass vessels.

Oxygen consumed by microorganisms from the oxidation of the test substance was continuously monitored by an automatic respirometer.

Test flasks were continuously stirred for 28 days. Test temperature was 22 +/- 1 Deg C.
Concentration-Nominal test concentration = 36 to 39mg/L for test substance.

Nominal concentration of the positive control (sodium benzoate) was 51 mg/L

Test substance : Dihexyl Phthalate (CAS# 68515-50-4)
(1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear)
Synonym: DHP

Conclusion : The substance is readily biodegradable.,

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

28.11.2000 (8)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	m >= .2 -
Method	:	other
Year	:	1982
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians. Statistical methods-Moving average angle, Probit or Bionomial
Result	:	Mean measured values used in calculation of LC50. Analytical samples taken at time zero and on a composite of replicates at termination. Measured values dropped slightly during the exposure period. One replicate of the second highest concentration exhibited toxicity. Fish mean Total length=62mm, mean wet weight=2.3g
Test condition	:	Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15L of solution. The diluter maintained a water turnover rate of 5-8 tank volumes per day. Two replicates of ten organisms were tested per treatment. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection. Test temperature=12 +/- 1 Deg C., The pH range was 7.2 to 7.5. The mean Dissolved Oxygen ranged from 9.2 to 9.4mg/L. Fish were obtained from Montana. Nominal test concentrations: control, 0.018, 0.036, 0.072, 0.14, and 0.29mg/L. Mean measured test concentrations: <0.0042, 0.014, 0.040, 0.057, 0.093, and 0.20mg/L.
Test substance	:	Dihexyl phthalate (CAS# 68515-50-4) (1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear) Synonym: DHP
Conclusion	:	Test substance is non-toxic to fish at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document 1.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

28.11.2000 (2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)

Unit	:	mg/l
Analytical monitoring	:	yes
EC50	:	m > .18 -
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975 Statistical methods-Moving average angle, Probit or Bionomial
Result	:	Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined to a level at or below the detection limit during study exposure. Lc50 value =>0.35ppm (based upon Day 0 analytical samples) was recalculated to >0.18 ppm as per USEPA current practices using mean of measured initiation and termination samples.
Test condition	:	Test treatments were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 30 minutes. The stock solution was prepared at the highest treatment concentration. Dilutions of the stock were prepared for each treatment level. Three replicates of five organisms were tested per treatment. Test vessels were 250ml beakers with 200ml of test solution. Analytical method was Gas Liquid Chromatography (GLC). Test temperature=22 +/- 2 Deg C., The pH was 8.3 to 8.6 at initiation and was from 8.3 at Day 2. Dissolved Oxygen ranged from 7.0 to 8.7 at initiation and 7.3 to 8.3 at Day 2. Daphnia were <24 hours old and obtained from in-house stock. Nominal test concentrations: control, 0.052, 0.086, 0.14, 0.24, and 0.40mg/L. Measured test concentrations <0.0083, 0.029, 0.048, 0.11, 0.20, and 0.41/0.29 (Day 0) Measured concentrations <0.0083, <0.0083, <0.0083, <0.0083, <0.0083, <0.0083, and 0.0084 mg/L (Day 2),
Test substance	:	Dihexyl phthalate (CAS# 68515-50-4) (1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear) Synonym: DHP
Conclusion	:	Test substance is non-toxic to Daphnia at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document 1.
Reliability	:	(2) valid with restrictions Loss of test substance during exposure. Loss of test substance during exposure.
Flag	:	Critical study for SIDS endpoint

18.06.2001 (1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	
Exposure period	:	7 day
Unit	:	mg/l
Analytical monitoring	:	yes
EC50	:	m > .33 -
Method	:	other

Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-EPA 600/9-78-018, Printz Algal Assay Bottle Test, 1978. Test type-Static Acute Statistical methods-Moving average angle, Probit or Bionomial
Result	:	In-vivo chlorophyll a, measured daily until less than 5% change. Both cell numbers and in-vivo chlorophyll a, measured at termination. Lowest test concentration showed a stimulatory effect as compared with the controls. Analytical samples taken at time zero and on a composite of replicates at termination.
Test condition	:	Test substance was added to Algal Growth Medium (control and diluent) to form a saturated phthalate solution and stirred for one hour and settled for one to two hours. After settling the test solution was drawn from the bottle and used as the secondary stock. This stock was diluted to achieve the actual test treatments. Initial algal concentration was 2.0x104 cells/ml. Lighting =4,500lux, Test temperature=24+/-1 Deg C. The pH range was 7.4 to 7.5 at initiation and 7.0 - 7.5 at day 7. Algal culture stock obtained from Univ. of Texas at Austin. Nominal test concentrations: 3.125, 6.25, 12.5, 25, 50, and 100 ppm. Measured test concentrations = 0.1, <0.1, 0.1, 0.1, 0.3, and 0.6 ppm (Day 0), Measured test concentration ND (Not Detected) on Day 7. Units-ppm Value-EC50=>0.6 ppm based upon Day 0 measured values only. Value recalculated as >0.33 ppm as per USEPA current practices using mean of measured initiation and termination samples 1.
Test substance	:	Dihexyl Phthalate (CAS# 68515-50-4) (1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear) Synonym: DHP
Conclusion	:	Test substance is not toxic to algae at or below its water solubility level.
Reliability	:	(1) valid without restriction Control chlorophyll or cell counts not reported.
Flag	:	Critical study for SIDS endpoint

18.06.2001 (3)

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	13 weeks (90 days)
Frequency of treatment	:	Daily for 13 weeks
Post obs. period	:	None
Doses	:	0, 0.05%, 0.1% and 0.5% (the 0.05% group was adjusted to 1.0% at 7 weeks and 3.0% at 12 weeks)
Control group	:	yes
NOAEL	:	= - .5 %
LOAEL	:	= - 3 %
Method	:	other
Year	:	1962
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	ANOVA; homogeneity of variance tested by method of Bartlett; differences from control y methods of Scheffe or Fischer-Behrens (modified t-test) Control Group: 10/sex/dose
Remark	:	Rats in the 0.05% group, which was increased to 1.0% at 7 weeks and 3.0% at 12 weeks displayed signs of respiratory distress, stiff gait, and rigidly or arched tail over the last three weeks of the study. Body weight gains and food consumption also were decreased for this group over that period. Total leukocyte counts were significantly increased for the 3.0% femalse at 90 days; blood chemistry, hematology and urinalysis values were comparable for all other groups and intervals. Heart/body weight ratios for mals in all three dose groups and thyroid weights for females in the 0.1% group were significantly increased over the controls. Rats of both sexes in the 3.0% group showed significantly increased liver weights and decreased spleen, kidneys, adrenals, and gonads weights. Microscopic examination tissues from rats in the 3.0% group revealed atrophy of the spermatogenic epithelium in th testes and slight changes in the liver characterized as eosinophilic areas in the cytoplasm and variation in the size of the nuclei.
Result	:	The NOAEL was 0.5% in the diet (approximately 383 mg/kg/day).The LOAEL was approximately 5.0%.
Test condition	:	Male and female rats were fed the test substance daily for 13 weeks at dietary levels of 0, 0.05%, 0.1% and 0.5%. The 0.5% group was increased to 1.0% at 7 weeks and 3.0% at 12 weeks. Clinical observations, body weights and food consumption were recorded weekly. Clinical blood chemistry, hematology, and urinalysis were performed on 5 rats/sex/group at 30 and 90 days. A complete necropsy was performed after 13 weeks and organ weights were recorded. Tissues from the control, 0.5% and 3.0% groups were examined microscopically.
Test substance	:	1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear (disohexyl phthalate)
Conclusion	:	Significant effects were found only at the highest dose tested (3%)
Reliability	:	(2) valid with restrictions

09.10.2001 (6)

Species	:	dog
Sex	:	male/female
Strain	:	Beagle
Route of admin.	:	oral feed
Exposure period	:	13 weeks (90 days)

Frequency of treatment	:	Daily
Post obs. period	:	None
Doses	:	0, 0.1, 0.5, or 1.0% (low dose adjusted to 5.0% during weeks 9-13)
Control group	:	yes
NOAEL	:	= - 1 %
LOAEL	:	= - 5 %
Method	:	other
Year	:	1962
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	All animals appeared normal in appearance and behavior throughout the study. No significant variations in weight were attributed to the test substance. Clinical blood chemistry, hematology, and urinalysis values were within normal limits and comparable to the controls, Mean liver weights and liver/body weight ratios for the dogs in the 5.0% group increased, and the males also exhibited decreased testes weight and ratio. Enlarged hepatic cells were observed in the males in the 5.0% group; these two males also exhibited atrophy of the seminiferous epithelium in the testes.
Result	:	The NOAEL was 1.0% (approximately 180 mg/kg/day).
Test condition	:	Male and female beagle dogs were fed the test substance daily for 13 weeks at dietary levels of 0.1, 0.5, or 1.0% (the 0.1% level was increased to 5.0% at week 9). The animals were observed daily; body weights and food consumption were recorded weekly. Hematology, blood chemistry, and urinalysis were performed initially and at 30 and 90 days. A complete necropsy was performed after 13 weeks. Organ weights were recorded and the tissues from the control and high dose groups were examined microscopically.
Test substance	:	1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear (diisohexyl phthalate)
Conclusion	:	Significant effects were found only at the highest dose tested (5%)
Reliability	:	(2) valid with restrictions

10.10.2001 (7)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	CD-1
Route of admin.	:	gavage
Exposure period	:	Single dose with sacrifices at 24, 48 and 72 hours.
Doses	:	0, 1250, 2500, and 5000 mg/kg
Result	:	negative
Method	:	OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year	:	1994
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Three groups of 5/sex/dose served as vehicle controls (corn oil) for the 24, 48, and 72 hour sacrifices; a single group of 5/sex/dose served as the positive control (cyclophosphamide) and was sacrificed at 24 hours. Statistical Methods: Analysis of variance (ANOVA) on proportion of cells with micronuclei per animal; Tukey's Studentized range test to determine which dose groups were different from the control.
Remark	:	The test substance induced no significant increases in micronucleated polychromatic erythrocytes over the levels observed in the concurrent vehicle control groups in eigher sex or at any sacrifice interval. The positive control group exhibited significant increases in both sexes.

Test condition : The test substance was solubilized in corn oil and dosed at a volume of 10 ml/kg. A total of 130 mice were used in the study; 15 sex/dose with 5/sex/dose sacrificed at 24, 48, or 72 hours after dosing. Bone marrow smears were prepared and stained after sacrifice. 1000 polychromatic erythrocytes (PCEs) per animal were scored for the incidence of micronucleated PCEs. The proportion of PCEs to normochromatic erythrocytes (NCEs) also was determined by counting a totoal of 1000 erythrocytes per animal.

Test substance : 1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear (disohexyl phthalate)

Conclusion : The test substance did not induce a statistically significant increase in bone marrow micronucleated polychromatic erythrocytes in male or female mice and was considered negative in this assay.

Reliability : (1) valid without restriction
18.06.2001 (9)

(1) CMA Study, Acute Toxicity of Fourteen Esters to Daphnia magna., Springborn Bionomics, Inc. 1984. Report # BW-84-4-1567.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(2) CMA Study, Acute Toxicity of Fourteen Esters to Rainbow Trout Salmo gairdneri Under Flow-Through Conditions. EG&G Bionomics, Inc. 1983. Report # BW-83-3-1373, Performed Jul 1982 to Jan 1983.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(3) CMA Study, Toxicity of Fourteen Esters to the Freshwater Green Alga Selenastrum capricornutum. 1984 by Springborn Bionomics, Inc. Performed 16-23 Mar 1983.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(4) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, Chemosphere 41:1389-1399.

(5) David, R., R. McKee, J. Butala, R. Barter and M. Kayser (2001), Chapter 80 - Esters of Aromatic Mono, Di and Tricarboxylic acids and Di, Tri, or Polyalcohols, Patty's Toxicology, 5th edition, Vol 6., J Wiley & Sons, Inc. pp 635-932.

(6) Esso Research and Engineering Company (1962). Dihexyl Phthalate: 90-Day dietary administration study in rats and dogs. Unpublished study.

(7) Esso Reshearch and Engineering Company (1962). Dihexyl Phthalate: 90-Day dietary administration study in rats and dogs. Unpublished study.

(8) Exxon Biomedical Sciences, Inc. Ready Biodegradability: Manometric Respirometry Test, Study Number 142994A, 1997 Exxon Biomedical Sciences, Inc.

(9) Exxonmobil Biomedical Sciences, Inc. (1994). In Vivo Mammalian Bone Marrow Micronucleus Assay. Unpublished study.

(10) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(11) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(12) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997), the Environmental Fate of Phthalate Esters: A literature Review, Chemosphere 35:667-749.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2, 3, 4 & 5

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 111381-90-9
CAS No.	:	111381-90-9
TSCA Name	:	1,2-Benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Synonym	:	1,2-benzenedicarboxylic acid (C7,C11) ester, branched and linear

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	05.11.2001
Revision date	:	
Date of last Update	:	05.11.2001
Number of Pages	:	12
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers:68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6, and 111381-90-9.

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from

alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate categories. Of the phthalates in this category, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

05.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

2.1 MELTING POINT

Value	:	-50 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	
Remark	:	Literature review collecting data from a variety of sources. Manufacturer's data or handbook value
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (6)

Value	:	85 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation Melting point calculation seems to give erroneously high results for the phthalate esters
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(3) invalid

08.10.2001 (5)

2.2 BOILING POINT

Value	:	440 - ° C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

08.10.2001 (5)

2.4 VAPOUR PRESSURE

Value	:	.000000068 - hPa at 25° C
Decomposition	:	no
Method		other (measured)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no

Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

08.10.2001 (1)

Value	:	.0000003 - hPa at 25° C
Decomposition	:	
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

08.10.2001 (5)

2.5 PARTITION COEFFICIENT

Log pow	:	8.6 - at 25° C
Method		other (measured)
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

15.12.2000 (1)

Log pow	:	9.37 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (5)

2.6.1 WATER SOLUBILITY

Value	:	.00002 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWIN ver 1.36 based on Kow correlation method of Meylan and Howard

Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

08.10.2001 (5)

Value	:	.00031 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

15.12.2000 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.0000000000248 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (5)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	6.2 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (5)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.0053
Water (level I)	:	0
Soil (level I)	:	97.7
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

Reliability : (2) valid with restrictions
15.12.2000 (4)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 2000
Result : Soil - 97.7%
Air - 0.0053%
Water - 0.000047%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (4)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Mouse lymphoma assay
System of testing	:	Mammalian Cell
Concentration	:	0.125 to 6 ml/ml.
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year	:	2000
GLP	:	yes
Test substance	:	other TS: 711P
Method	:	Control Group: The negative control article was the solvent (acetone) used in the assay. Ethylmethane sulfonate (EMS) was used as a positive control in the assays without S9 activation. 3-methylcholanthrene which requires metabolic activation, was used as a positive control for assays with S9. Statistical Methods: The minimum criterion necessary to demonstrate mutagenesis was a mutation frequency that was at least 1.5 times the concurrent background frequency plus 10 x 10-6. The background frequency was defined as the average mutant frequency of the solvent negative controls.
Result	:	In the absence of activation, 0.75 to 6.0 ul/ml induced moderate to high toxicity (percent relative growths: 3.2% to 48.4%), but only a slight increase in mutation frequency at the highest doses. In the presence of a metabolic fraction, 0.125 to 1.5 ul/ml resulted in percent relative growths of 8.9% to 82.2% without increasing the incidence of mutations. Thus, the test compound was considered non-mutagenic in this assay.
Test condition	:	Mouse lymphoma cells were seeded into a series of tubes at 6 x 106 cells per tube. Dosed tubes were exposed for 4 hours to the test substance. An expression period of 48 hours was used; after the 48 hour expression time, 3 x 106 cells per plate were added to semi-solid selection medium containing 3 ug/ml trifluorothymidine (TFT) to score for mutant colonies and 200 cells per plate were added to cloning medium, without TFT, to evaluate viability. Mutant frequencies were calculated after 10-14 days incubation. Mutant and total colony count at each dose level were determined by triplicate plates.
Test substance	:	Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11). Data used as read-across to 1,2-benzenedicarboxylic acid, heptyl undecyl ester. CAS# 111381-90-9.
Conclusion	:	Under conditions of this study the test substance was non-mutagenic in the mouse lymphoma assay with or without metabolic activation.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

05.11.2001 (2)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female

Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	Gestation days 6-15
Frequency of treatment	:	Daily
Duration of test	:	9 days
Doses	:	0, 40, 200, 1000 mg/kg/day.
Control group	:	yes, concurrent vehicle
NOAEL Maternalt.	:	= - 200 mg/kg bw
NOAEL Teratogen	:	= - 200 mg/kg bw
Method	:	OECD Guide-line 414 "Teratogenicity"
Year	:	1997
GLP	:	yes
Test substance	:	other TS: 711P
Method	:	Statistical Methods: Dunnett's Test for food consumption, body weight, organ weight, placental and fetal data; Fisher's Exact Test for female mortality, litters with findings; and the Wilcoxon Test for proportion of fetuses with findings per litter.
Result	:	Maternal Effects: There were no treatment-related effects in the 40 or 200 mg/kg/day groups either in the dams or fetuses. The high dose (1000 mg/kg/day) maternal body weights were decreased during gestation days 15-20, and relative liver and kidney weight was increased in the high dose group dams. Six of the ten high dose dams showed vaginal hemorrhage during the study; three had complete resorptions. Embryo/Fetal Effects: Fetal weights of the remaining viable litters were reduced, and all litters contained malformations. The malformations affected mainly the brain, vertebral column, tail, scapula, sternum, and urogenital tract. In total, 47/53 high-dose fetuses (89%) from all seven litters were malformed.
Test condition	:	Eight to ten pregnant females were used per group. Animals were weighed on gestation days 0, 6, 10, 15, and 20, and observed daily for signs of toxicity. On GD 20, animals were sacrificed and maternal body, liver, kidneys, and intact uterus were weighed. Fetuses were weighed, examined for external and visceral abnormalities.
Test substance	:	Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11). Data used as read-across to 1,2-benzenedicarboxylic acid, heptyl undecyl ester. CAS# 111381-90-9.
Conclusion	:	Significant maternal and fetal effects only were observed at the high dose (1000 mg/kg/day). No treatment-related effects were observed in the 40 or 200 mg/kg/day groups.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

05.11.2001 (3)

6. References

(1) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, Chemosphere 41:1389-1399.

(2) E. Barber, M. Cifone, J. Rundell, R. Przygoda, B. Astill, E. Moran, A. Mulholland, E. Robinson and B. Schneider. (1999). Results in the L5178Y mouse lymphoma and the in vitro transformation of Balb 3T3 cell assays for eight phthalate esters. Journal of Applied Toxicology 20:69-80.

(3) J. Hellwig, H. Freudenberger and R. Jackh. (1997). Differential prenatal toxicity of branched phthalate esters in rats. Food and Chemical Toxicology 35:501-512.

(4) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(5) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(6) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997), the Environmental Fate of Phthalate Esters: A literature Review, Chemosphere 35:667-749.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2, 3, 4 & 5

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 71888-89-6
CAS No.	:	71888-89-6
EINECS Name	:	Diisoheptyl phthalate
EINECS No.	:	276-158-1
Molecular Weight	:	362
Molecular Formula	:	C22H34O4

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - transitional phthalates
Printing date	:	06.11.2001
Revision date	:	
Date of last Update	:	06.11.2001
Number of Pages	:	14
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers:68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6, and 111381-90-9.

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from

alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate categories. Of the phthalates in this category, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

05.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

2.1 MELTING POINT

Value	:	-45 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	
Remark	:	Manufacturer's data or handbook value
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

06.11.2001 (2)

Value	:	43 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	other: calculated
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Melting point calculation by MPBBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation Melting point calculation seems to give erroneously high results for the phthalate esters
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(3) invalid

05.11.2001 (9)

2.2 BOILING POINT

Value	:	398 - ° C at 1013 hPa
Decomposition	:	no
Method	:	other: calculated value
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Boiling point calculation by MPBBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

06.11.2001 (9)

Value	:	>300 ° C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Manufacturer's data or handbook value.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(4) not assignable

06.11.2001 (2)

2.4 VAPOUR PRESSURE

Value	:	.000000933 - hPa at 25° C
Decomposition	:	no
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Decomposition	:	no
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (1)

Value	:	.0000108 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Boiling point calculation by MPBBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (9)

2.5 PARTITION COEFFICIENT

Log pow	:	6.87 - at 25° C
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

14.12.2000 (1)

Log pow	:	7.41 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (9)

2.6.1 WATER SOLUBILITY

Value	:	.00245 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

05.11.2001 (9)

Value	:	.02 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

14.12.2000 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.00000000001774 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (9)

3.1.2 STABILITY IN WATER

Type	:	
t1/2 pH4	:	- at degree C
t1/2 pH7	:	3.4 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

14.12.2000 (9)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.138
Water (level I)	:	.0043
Soil (level I)	:	97.6
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

14.12.2000 (6)

3.3.2 DISTRIBUTION

Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level I
Year	:	2000
Result	:	Soil - 97.6% Air - 0.138% Water - 0.00429% Sediment - 2.169% Suspended sed. - 0.068%
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

14.12.2000 (6)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	Wistar
Sex	:	male
Number of animals	:	35
Vehicle	:	no data
Value	:	> - 10000 mg/kg bw
Method	:	other
Year	:	1978
GLP	:	no data
Test substance	:	other TS
Remark	:	There were no deaths at any dose level or time point. Signs of toxicity included diarrhea, lethargy and piloerection. At all dose levels, these signs were observed in the early stages of the test. Most of these signs were diminished during the later part of the observation period.
Test condition	:	Seven groups (5 per group) of male Wistar rats at least 8 weeks of age were dosed with diisoheptyl phthalate by syringe at doses of 1.0, 1.47, 2.15, 3.16, 4.64, 6.81 and 10.0 g/kg. The rats were observed at 1, 2, 4 and 6 hours after dosing and once daily for 14 days. Mortality, toxicity and pharmacological effects were recorded. On day 14, the survivors were sacrificed. All animals were examined for gross pathology
Test substance	:	1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (diisoheptyl phthalate)
Conclusion	:	The test material was not acutely toxic at levels up to 10.0 g/kg.
Reliability	:	(2) valid with restrictions

02.01.2001 (8)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	2
Vehicle	:	
Value	:	= - 3160 mg/kg bw
Method	:	other (calculated)
Year	:	1979
GLP	:	no
Test substance	:	other TS
Remark	:	There were no deaths at the tested dose level. Slight erythema was noted at the 24 hour observation only. At necropsy, all animals were observed with dilated hearts.
Test condition	:	A single dose level of 3160 mg/kg body weight was used. On the day prior to dosing the fur of each rabbit was clipped from the abdomen. The skin also was abraded. The test material was applied directly to the skin and the area was wrapped with gauze and an impervious plastic sleeve. The wraps were removed after 24 hours and dermal observations recorded. General observations were recorded immediately after dosing, 2 and 4 hours; and once daily thereafter for 14 days. Observations for skin irritation were recorded 30 minutes after removal of the wrap and at Days 3, 7, 10, and 14. Body weights were recorded prior to dosing and at 14 days.

Gross necropsies were conducted on all animals that were sacrificed at the termination of the study.

Test substance : 1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (diisoheptyl phthalate)

Conclusion : The test material was not acutely toxic at levels up to 3.16 g/kg.

Reliability : (2) valid with restrictions

10.10.2001 (7)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test

System of testing : Bacterial

Concentration : 250, 500, 1000, 2500, and 5000 mg/ml

Cycotoxic conc. :

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"

Year : 1995

GLP : yes

Test substance : other TS

Method : Statistical Methods: The mean revertant colony count and standard deviation were determined for each dose point (Snedecor and Cochran, 1989). An individual dose was considered positive if the mean revertant count on the test plates was equal to or greater than three times the mean number of spontaneous revertants on the vehicle control plates.

Result : In both the initial and repeat assays the test substance beaded on the plate at concentrations of 500 mg/plate and greater. However, the test substance was soluble in the vehicle, DMSO. The test material did not induce a significant difference in revertant colonies in tester strains TA 98, TA100, TA 1535, TA1537 or TA1538 at any dose level with or without metabolic activation in either the initial or repeat assays.

Test condition : Prior to assay initiation, a toxicity pretest was performed using tester strain TA98. Based on these results, the doses for the final assay were determined. In the definitive assay, each of the four strains was dosed either with the test substance; a vehicle control (DMSO); or a nontreated control and a positive control. Positive controls were as follows: 2-aminoanthracene (all strains with S9); 2-nitrofluorene (TA 98, TA1538 without S9); N-methyl-n-nitro-n-nitrosoguanidine (TA 100, TA 1535 without S9) and 9-aminoacridine (TA1537 without S9). There were 3 plates/dose group/strain/treatment. The test results were verified by repeating the assay. Both the initial and repeat assays were terminated approximately 48 hours following dose initiation.

Test substance : 1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (diisoheptyl phthalate)

Conclusion : Under conditions of this study, diisoheptyl phthalate was inactive in the Ames mutation assay.

Reliability : (1) valid without restriction

02.01.2001 (3)

Type : Chromosomal aberration test

System of testing : Non-Bacterial

Concentration : 499, 1250, 2500, 3750, and 4990 mg/ml

Cycotoxic conc. :

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 473 "Genetic Toxicology: In vitro Mammalian Cytogenetic Test"

Year : 1991

GLP	:	yes
Test substance	:	other TS
Method	:	Statistical Methods: A statistically significant (P < 0.05) difference for one dose point and a significant trend (P < 0.015) were considered evidence of a positive response; significant differences for two or more doses indicated the trial was positive.
Result	:	In the 10 hour harvest assay, no significant increase in cells with chromosomal aberrations was observed at the doses analyzed. Similarly, no significant increase in cells with chromosomal aberrations was observed in the 20 hour assay. Evidence that the metabolic system was working properly was demonstrated by the cyclophosphamide-induced increased incidence in aberrations.
Test condition	:	Results from a rangefinding assay were used to determine the dose range used in the study. In the rangefinding assay, the cultures were incubated for 25-26 hours with 5-bromo-2'deoxyuridine. In the chromosomal aberration assay, replicate cultures were used at each dose level. Single cultures were used for the negative controls, solvent control, and at each of two doses of the positive control. Solvent controls were cultures containing the solvent for the test material. The positive controls used in this assay were: mitomycin C(without S9) and cyclophosphamide (with S9). In the assay without S9, a harvest time of 20 hours was used. In the assay with S9, harvest times of 10 and 20 hours were used.
Test substance	:	1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (diisoheptyl phthalate)
Conclusion	:	No induction of chromosomal aberrations was observed in CHO cells in the presence or absence of S9.
Reliability	:	(1) valid without restriction

02.01.2001 (5)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Gestation days 6-15
Frequency of treatment	:	Daily
Duration of test	:	9 days
Doses	:	0, 100, 300, or 750 mg/kg/day.
Control group	:	yes
NOAEL Maternalt.	:	= - 750 mg/kg bw
NOAEL Teratogen	:	= - 300 mg/kg bw
Method	:	OECD Guide-line 414 "Teratogenicity"
Year	:	1997
GLP	:	yes
Test substance	:	other TS
Method	:	ANOVA; Dunnett's Test; Dunn's Summed Rank Test.
Result	:	Maternal Effects: There were dose-related increases in mean absolute and relative maternal liver weights that were statistically significant in the 300 and 750 mg/kg dams compared with controls. These increases were consistent with the known ability of certain other alkyl esters of 1,2-benzenedicarboxylic acid to cause peroxisome proliferation and were considered to be a physiological adaptation. Thus, under the condition of this study, no clear maternal toxicity was identified. Embry/fetal Effects: At doses of 300 mg/kg or less, there were no treatment-related or biologically important fetal malformations, embryolethality, or fetal weight reduction. Evidence of growth retardation

and increased embryo/fetal death was observed in the high dose (750 mg/kg) group compared with controls. Additionally, there was an increased incidence of external, visceral and skeletal malformations/variations in the 750 mg/kg compared with control.

Test condition : The test material was administered by oral gavage to 25 confirmed-mated female rats at doses of 0 (corn oil only), 100, 300, and 750 mg/kg at a dose volume of 5 ml/kg once daily from gestation day (GD) 6 through GD 20. Clinical observations were made daily during gestation. Body weight and food consumption measurements were made on GD 0, 6, 9, 12, 15, 18, and 21. On GD 21, animals were sacrificed and cesarean sections were performed. Gross necropsies were performed, liver weights and uterine weights with ovaries attached were recorded, uterine contents were examined, and the required uterine implantation data were recorded. All live fetuses were weighed, sexed externally, and examined externally for gross malformations.

Test substance : 1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (diisoheptyl phthalate)

Conclusion : Under the conditions of this study the test material was considered embryolethal, fetotoxic, and a selective developmental toxicant at a dose of 750 mg/kg.

Reliability : (1) valid without restriction

02.01.2001 (4)

6. References

(1) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, Chemosphere 41:1389-1399.

(2) David, R., R. McKee, J. Butala, R. Barter and M. Kayser (2001), Chapter 80 - Esters of Aromatic Mono, Di and Tricarboxylic acids and Di, Tri, or Polyalcohols, Patty's Toxicology, 5th edition, Vol 6., J Wiley & Sons, Inc. pp 635-932.

(3) Exxon Biomedical Sciences, Inc. (1995). Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay. Project No. 167634. Unpublished report.

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(5) Hazleton Laboratories America, Inc. (1991). Mutagenicity Test in an In Vitro Cytogenetic Assay. Project No. 181232. Conducted for Exxon Biomedical Sciences, Inc. Unpublished report.

(6) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(7) MB Research Laboratories (1979). Test for dermal toxicity in rabbits. Project no. MB 79-3967. Conducted for Exxon Biomedical Sciences, Inc. Unpublished report.

(8) MB Research Laboratories (1979). Test for oral toxicity in rats. Project No. MB 79-3967. Conducted for Exxon Biomedical Sciences, Inc. Unpublished report.

(9) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2, 3, 4 & 5

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

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7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 111381-89-6
CAS No.	:	111381-89-6
TSCA Name	:	1,2-Benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Synonym	:	1,2-benzenedicarboxylic acid (C7-C9) ester, branched and linear

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	06.11.2001
Revision date	:	
Date of last Update	:	05.11.2001
Number of Pages	:	11
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

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1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers:68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6, and 111381-90-9.

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from

alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate categories. Of the phthalates in this category, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

05.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

2.1 MELTING POINT

Value	:	-45 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	
Remark	:	Manufacturer's data or handbook value
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(4) not assignable

15.12.2000 (1)

Value	:	64 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation Melting point calculation seems to give erroneously high results for the phthalate esters
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(3) invalid

10.10.2001 (5)

2.2 BOILING POINT

Value	:	417 ° C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (5)

Value	:	> 300 ° C at 1013 hPa
Decomposition	:	no
Method	:	other (measured)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Manufacturer's data or handbook value.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(4) not assignable

10.10.2001 (1)

2.4 VAPOUR PRESSURE

Value	:	.00000185 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (5)

2.5 PARTITION COEFFICIENT

Log pow	:	8.39 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (5)

2.6.1 WATER SOLUBILITY

Value	:	.00024 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (5)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.000000000022 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (5)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	4.2 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (5)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.027
Water (level I)	:	.0005
Soil (level I)	:	97.7
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

Reliability : (2) valid with restrictions
15.12.2000 (4)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 2000
Result : Soil - 97.7%
Air - 0.027%
Water - 0.00045%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (4)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Mouse lymphoma assay
System of testing	:	Mammalian cell
Concentration	:	0.125 to 6 ul/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year	:	2000
GLP	:	yes
Test substance	:	other TS: 711P
Method	:	Control Group: The negative control article was the solvent (acetone) used in the assay. Ethylmethane sulfonate (EMS) was used as a positive control in the assays without S9 activation. 3-methylcholanthrene which requires metabolic activation, was used as a positive control for assays with S9. Statistical Methods: The minimum criterion necessary to demonstrate mutagenesis was a mutation frequency that was at least 1.5 times the concurrent background frequency plus 10 x 10-6. The background frequency was defined as the average mutant frequency of the solvent negative controls.
Result	:	In the absence of activation, 0.75 to 6.0 ul/ml induced moderate to high toxicity (percent relative growths: 3.2% to 48.4%), but only a slight increase in mutation frequency at the highest doses. In the presence of a metabolic fraction, 0.125 to 1.5 ul/ml resulted in percent relative growths of 8.9% to 82.2% without increasing the incidence of mutations. Thus, the test compound was considered non-mutagenic in this assay.
Test condition	:	Mouse lymphoma cells were seeded into a series of tubes at 6 x 106 cells per tube. Dosed tubes were exposed for 4 hours to the test substance. An expression period of 48 hours was used; after the 48 hour expression time, 3 x 106 cells per plate were added to semi-solid selection medium containing 3 ug/ml trifluorothymidine (TFT) to score for mutant colonies and 200 cells per plate were added to cloning medium, without TFT, to evaluate viability. Mutant frequencies were calculated after 10-14 days incubation. Mutant and total colony count at each dose level were determined by triplicate plates.
Test substance	:	Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11). Data used as read-across to 1,2-benzenedicarboxylic acid, heptyl nonyl ester. CAS# 111381-89-6.
Conclusion	:	Under conditions of this study the test substance was non-mutagenic in the mouse lymphoma assay with or without metabolic activation.
Reliability	:	(1) valid without restriction

05.11.2001 (2)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female

Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	9 days
Frequency of treatment	:	daily
Duration of test	:	20 days
Doses	:	0, 40, 200, 1000 mg/kg/day
Control group	:	yes, concurrent vehicle
NOAEL Maternalt.	:	= 200 - mg/kg bw
NOAEL Teratogen	:	= 200 - mg/kg bw
Method	:	Control Group: Yes, Olive Oil Vehicle control Statistical Methods: Dunnett's Test for food consumptionm body weight, organ wight, placental and fetal data; Fisher's Exact Test for female mortality, litters with findings; and the Wilcoxon Test for proportion of fetuses with findings per litter.
Result	:	Maternal effects: There were no treatment-related effects in the 40 or 200 mg/kg/day groups either in the dams or fetuses. The high dose (1000 mg/kg/day) maternal body weights were decreased during gestation days 15-20, and relative liver and kidney weight was increased in the high dose group dams. Six of the ten high dose dams showed vaginal hemorrhage during the study; three had complete resorptions. Embryo/fetal effects: Fetal weights of the remaining viable litters were reduced, and all litters contained malformations. The malformations affected mainly the brain, vertebral column, tail, scapula, sternum, and urogenital tract. In total, 47/53 high-dose fetuses (89%) from all seven litters were malformed.
Test condition	:	Eight to ten pregnant females were used per group. Animals were weighed on gestation days 0, 6, 10, 15, and 20, and observed daily for signs of toxicity. On GD 20, animals were sacrificed and maternal body, liver, kidneys, and intact uterus were weighed. Fetuses were weighed, examined for external and visceral abnormalities.
Test substance	:	Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11). Data used as read-across to 1,2-benzenedicarboxylic acid, heptyl nonyl ester. CAS# 111381-89-6.
Conclusion	:	Significant maternal and fetal effects only were observed at the high dose (1000 mg/kg/day). No treatment-related effects were observed in the 40 or 200 mg/kg/day groups.

05.11.2001 (3)

6. References

(1) David, R., R. McKee, J. Butala, R. Barter and M. Kayser (2001), Chapter 80 - Esters of Aromatic Mono, Di and Tricarboxylic acids and Di, Tri, or Polyalcohols, Patty's Toxicology, 5th edition, Vol 6., J Wiley & Sons, Inc. pp 635-932.

(2) E. Barber, M. Cifone, J. Rundell, R. Przygoda, B. Astill, E. Moran, A. Mulholland, E. Robinson and B. Schneider. (2000). Results in the L5178Y mouse lymphoma and the in vitro transformation of Balb 3T3 cell assays for eight phthalate esters. Journal of Applied Toxicology 20:69-80.

(3) J. Hellwig, H. Freudenberger and R. Jackh. (1997). Differential prenatal toxicity of branched phthalate esters in rats. Food and Chemical Toxicology 35:501-512.

(4) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(5) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2, 3, 4 & 5

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

I U C L I D

D a t a s e t

Existing Chemical	Substance ID: 85-68-7
CAS No.	85-68-7
EINECS Name	benzyl butyl phthalate
EINECS No.	201-622-7
Molecular Formula	C19H20O4

Dataset created by: EUROPEAN COMMISSION - European Chemicals Bureau

This dossier is a compilation based on data reported by the European Chemicals Industry following 'Council Regulation (EEC) No. 793/93 on the Evaluation and Control of the Risks of Existing Substances'. All (non-confidential) information from the single datasets, submitted in the IUCLID/HEDSET format by individual companies, was integrated to create this document.

The data have not undergone any evaluation by the European Commission.

Creation date: 19-FEB-2000

Number of Pages: 90

Chapters: all

Edition: Year 2000 CD-ROM edition

Flags: non-confidential

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European Chemicals Bureau

1.0.1 OECD and Company Information

Name: Alusuisse Italia Spa
Street: via del Pruneto, 40
Town: I-52027 S.Giovanni Valdarno (AR)
Country: Italy
Phone: 055/940032
Telefax: 055/943936
Telex: 570447

Name: Bayer AG
Town: 51368 Leverkusen
Country: Germany

Name: Enichem S.p.A.
Street: Via Taramelli,26
Town: 20124 Milan
Country: Italy

Name: Monsanto Europe N.V.
Street: Tervurenlaan, 270-272
Town: 1150 Bruxelles
Country: Belgium

Name: Morton International Limited
Street: 155-157 Staines Road
Town: MIDDX TW3 3 JB Hounslow
Country: United Kingdom

1.0.2 Location of Production Site

-

1.0.3 Identity of Recipients

-

1.1 General Substance Information

Substance type: organic
Physical status: liquid

1.1.1 Spectra

-

1.2 Synonyms

1,2-benzenedicarboxylic acid, butyl phenylmethyl ester
Source: Monsanto Europe N.V. Bruxelles

1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester
Source: Morton International Limited Hounslow

1,2-Benzenedicarboxylic acid; butyl phenylmethyl ester; BBP; benzyl butylphthalate; Sicol 160
Source: Enichem S.p.A. Milan

BBP
Source: Morton International Limited Hounslow

benzyl butyl phthalate
Source: Monsanto Europe N.V. Bruxelles
Bayer AG Leverkusen

benzyl-n-butyl phthalate
Source: Monsanto Europe N.V. Bruxelles
Bayer AG Leverkusen

Butilbenzilftalato
Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

Diplast BBP
Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

phthalic acid, butyl benzyl ester
Source: Bayer AG Leverkusen

phthalic acid,butyl benzyl ester
Source: Monsanto Europe N.V. Bruxelles

Santicizer 160
Source: Monsanto Europe N.V. Bruxelles

Sicol 160
Source: Monsanto Europe N.V. Bruxelles

Unimoll BB
Source: Monsanto Europe N.V. Bruxelles

Source: Monsanto Europe N.V. Bruxelles

1.3 Impurities

-

1.4 Additives

-

1.5 Quantity

Quantity 100 000 - 500 000 tonnes

1.6.1 Labelling

-

1.6.2 Classification

-

1.7 Use Pattern

Type: type
Category: Use resulting in inclusion into or onto matrix

Type: industrial
Category: Paints, lacquers and varnishes industry

Type: industrial
Category: Polymers industry

Type: use
Category: other: Plasticisers

Type: use
Category: other: plasticizer

Type: use
Category: other: plasticizer/polymer additive

Type: use
Category: other: plastificante

1.7.1 Technology Production/Use

-

1.8 Occupational Exposure Limit Values

Type of limit: other: PRODUCER-GUIDELINE
Limit value: 5 mg/m3
Remark: Guidance value is generic for phthalate esters and is not health-based.
Saturated vapour concentrations at 20 deg.C would be very much less than 5mg/m3.
Since aerosol production does not occur in manufacturing,work-place air concentrations have not been measured.
Source: Monsanto Europe N.V. Bruxelles

Type of limit:
Limit value:
Remark: No assigned TLV
Source: Enichem S.p.A. Milan

(1)

1.9 Source of Exposure

Remark: Butyl benzyl phthalate is used mainly in a variety of specialty engineering and commodity polymers to modify the hardness/softness and flexibility of the finished product.
Polyvinyl chloride(PVC) is by far the largest volume user of these polymer modifiers.

Major end-uses are in flooring,sealants,auto industry components and other engineering/construction materials based on PVC.
Two different methods are used to physically incorporate plasticizers into PVC-dry blending and plastisol technology.The dry blend or,plastisol,is subsequently subjected to heat in order to melt/cure the polymer during the calendering ,or coating process.
Coating lines are now widely fitted with fitration and oven exhaust incineration systems and several industry studies(Ref 1,2) have shown that emissions to the environment from this source are now considered minimal.
For example,Berndtsson(1991) in a study of Swedish spread coating/plastisol processing lines estimated the phthalate emission at 0.08% of total phthalate ester usage.
Another industry study(Ref 2) estimated the total European emission from spread coating lines with filtration/incineration equipment(estimated 75%) at 40 tonnes per year.

Other potential sources of exposure or environmental entry are from product manufacture,bulk transport operations,and/or converter end-use sites following tank washing and waste-water effluent treatment.Also from leaching upon disposal (mainly landfill) of plastic components.

The ready biodegradability of BBP under both aerobic and anaerobic conditions would preclude accumulation in the environment from either of these routes of entry(Ref 3).

Data from several environmental monitoring studies in the United States,Canada,and W.Europe(Rhine basin)support the conclusion that high levels of exposure to BBP ,or phthalate esters in general,has not been demonstrated ,and that widespread concentrations are not present in the environment.(Ref 4).
Measured concentrations fall well below those predicted from modelling undoubtedly due to this materials ready biodegradability.

Source: Monsanto Europe N.V. Bruxelles

(2)

Remark: Diffusions of BBP from consumer products is expected to be minimal. Other possible sources of BBP release to the environment are from its manufacture, distribution, and from PVC blending operations.

Source: Enichem S.p.A. Milan

(3)

Remark: La sostanza in esame è prodotta nello Stabilimento Enichem di Porto Marghera per conto dell'Alusuisse Italia SPA. Il processo è di tipo discontinuo (per batch) e consiste essenzialmente nelle seguenti fasi:

- Reazione
- Purificazione
- Filtrazione

Tutte le fasi del processo vengono condotte a ciclo chiuso in quanto tutte le sostanze coinvolte nella sintesi chimica sono movimentate attraverso pompe , tubazioni, sistemi di trasferimento e apparecchiature di tipo chiuso.
Gli effluenti del processo sono i seguenti:
1) Acqua di reazione
2) Gas incondensabili

L'acqua di reazione, contenente tracce di sostanze organiche, viene raccolta e trasferita al trattamento di depurazione nell'impianto chimico biologico, quindi immessa in acque superficiali secondo i limiti stabiliti dalle leggi nazionali (Legge Merli n°319/76).
I gas incondensabili vengono immessi in atmosfera in conformità alle leggi nazionali vigenti (DPR 203/88).

Dati relativi alle emissioni

Acque trattate :

* tipo di emissione - puntiforme
* Durata emissione - continua

Emissioni atmosfera:

* tipo di emissione - puntiforme
* Portata - 15 Nm3/h per Ton. di prodotto
* durata emissione - continua

Fattori potenziali di esposizione umana
La sostanza ha un'elevata temperatura di ebollizione ed una bassissima tensione di vapore; si ritiene insignificante il potenziale di esposizione ai vapori da parte dell'utilizzatore del manufatto plastico/elastomerico dove la sostanza è presente in percentuali varabili.

Settori di impiego
La sostanza fa parte della famigia dei plastificanti che costituiscono gli additivi per materie plastiche ed elastomeri, migliorandone la flessibilità e la lavorabilità.

La maggior parte dei plastificanti sono addizionati al PVC per trasformarlo in una varietà di materiali con caratteristiche diversificate, dal semirigido all'estremamente fessibile.

Processi relativi ai settori di impiego

La sostanza viene miscelata agli altri componenti del manufatto in apparecchiature di tipo chiuso, quindi la mescola ottenuta viene inviata allo stampaggio, effettuato a caldo (80-200 °C) in apparecchiature dotate di impianti localizzati di aspirazione.

Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

1.10.1 Recommendations/Precautionary Measures

-

1.10.2 Emergency Measures

-

1.11 Packaging

-

1.12 Possib. of Rendering Subst. Harmless

-

1.13 Statements Concerning Waste

-

1.14.1 Water Pollution

-

1.14.2 Major Accident Hazards

-

1.14.3 Air Pollution

-

1.15 Additional Remarks

Source: Monsanto Europe N.V. Bruxelles

Remark: Possibilità di eliminazione

La sostanza ha una bassa solubilità in acqua (2.9 mg/l).
Il manufatto a base di PVC può essere riciclato o eliminato in appositi impianti di incenerimento con recupero energetico e controllo emissioni all'atmosfera o smaltito in discarica come rifiuto solido urbano secondo la normativa vigente (DPR 915/82)

Informazioni sul trasporto

La sostanza, stoccata in serbatoi fuori terra, può essere spedita alla rinfusa con autobotti o in fusti da 220 litri.

Trasporto su strada (nazionale/Internazionale)

- Tipo del mezzo: Autobotte/ autocisterna per prodotti non ADR

- Quantità media trasportata : 23.000 Kg (autobotti/autocisterna)
  16.000 Kg (containers)

- Automezzi/mese : 10/30

- Misure di controllo durante il trasporto:

Il prodotto viaggia con la documentazione stabilita dalle leggi vigenti in materia. Nonostante non sia previsto dalle normativa, in quanto prodotto non pericoloso ai fini del trasporto, viene consegnata all'autista una scheda, tipo TREM CARD, con notizie utili al soccorso stradale, in caso di incidente.

Trasporto via mare

- Il prodotto è classificato " Marine polluttant " UN n° 3077 classe 9. Gli imballi vengono quindi etichetttati e il carico accompagnato con i previsti documenti di sicurezza.

Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

1.16 Last Literature Search

-

1.17 Reviews

-

1.18 Listings e.g. Chemical Inventories

-

2.1 Melting Point

Value: < -35 degree C
Decomposition: no
Sublimation: no
Method: other
GLP: no data
Remark: NOTE:Crystallising Point < -35 degrees C
Source: Monsanto Europe N.V. Bruxelles

(4) (5)

2.2 Boiling Point

Value: = 235 - 255 degree C at 13 hPa
Method: other
GLP: no data
Source: Monsanto Europe N.V. Bruxelles

(6)

Value: ca. 370 degree C at 10.13 hPa
Decomposition: no
Method: other
GLP: no data
Source: Monsanto Europe N.V. Bruxelles

(7)

2.3 Density

Type: density
Value: = 1.114 - 1.122 g/cm3 at 25 degree C
Method: other
Year: 1993
GLP: no data
Source: Monsanto Europe N.V. Bruxelles

(8)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: = .00000041 hPa at 20 degree C
Method: OECD Guide-line 104 "Vapour Pressure Curve"
Year: 1987
GLP: no data
Source: Monsanto Europe N.V. Bruxelles

(9)

Value: = .0000008 hPa at 25 degree C
Method: OECD Guide-line 104 "Vapour Pressure Curve"
Year: 1987
GLP: no data
Source: Monsanto Europe N.V. Bruxelles

(10)

Value: = .016 hPa at 150 degree C
Method: other (measured)
Year: 1977
GLP: yes
Source: Monsanto Europe N.V. Bruxelles

(11)

Value: = .192 hPa at 250 degree C
Method: other (measured)
GLP: yes
Source: Monsanto Europe N.V. Bruxelles

(12)

2.5 Partition Coefficient

log Pow: = 3.57
Method:
Year: 1985
GLP: yes
Remark: Measured
Source: Monsanto Europe N.V. Bruxelles

(13)

log Pow: = 4.78
Method:
Year:
GLP: yes
Remark: Measured
Source: Monsanto Europe N.V. Bruxelles

(14)

log Pow: = 4.91
Method:
Year:
GLP: yes
Remark: Measured
Source: Monsanto Europe N.V. Bruxelles

(15)

2.6.1 Water Solubility

Value: = .71 mg/l at 25 degree C
Method: other: Nephelometric
Year: 1979
GLP: no data
Source: Monsanto Europe N.V. Bruxelles

(16)

Value: = 2.69 mg/l at 25 degree C
Method: other
Year: 1985
GLP: yes
Source: Monsanto Europe N.V. Bruxelles

(17)

2.6.2 Surface Tension

-

2.7 Flash Point

Value: > 215 degree C
Type:
Method: other: DIN51794
Year:
GLP: yes
Source: Monsanto Europe N.V. Bruxelles

(18) (8)

2.8 Auto Flammability

-

2.9 Flammability

-

2.10 Explosive Properties

-

2.11 Oxidizing Properties

-

2.12 Additional Remarks

Source: Monsanto Europe N.V. Bruxelles

3.1.1 Photodegradation

Type: water
Light source: Sun light
Conc. of subst.: 1 mg/l at 24 degree C
DIRECT PHOTOLYSIS
Halflife t1/2: > 100 day
Degradation: < 5 % after
Method: other (measured): American Society for Testing Materials, Proposed StandardPractice for Conducting Aqueous Photolysis Test, Draft No. 5, ASTM E35.24Subcommittee, Aqueous Photolysis Task Group.
Year: 1979 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Test condition: The sunlight exposure took place on the 28 days between August 20 and September 17, 1979. During this period, there were approximately 251 hours of sunshine which is 70% of the maximum possible. The average air temperature was 85 degrees F and the average minimum was 65 degrees F. The latitude was 38 degrees 37 minutes and 44 seconds.

(19)

Type: water
Light source: Sun light
Conc. of subst.: 1 mg/l at 24 degree C
DIRECT PHOTOLYSIS
Halflife t1/2: > 10 day
Degradation: < 5 % after 10 day
Method: other (measured): "Draft guidance for Premanufacturing Notification"
Year: 1978 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Not susceptible to direct photolysis; data was as follows: day 0 0.832 mg/l, day 0.25 0.833, day 2 0.829, day 10 0.895 and day 28 0.442.
Source: Monsanto Europe N.V. Bruxelles
Test condition: Sunlight exposure took place on the 28 days between August 29 and September 26, 1978. During this period there were approximately 252 hours of sunshine which is 71% of the maximum possible. The average maximum air temperature was 30C and the average minimum was 17C. The test was carried out in St. Louis MO USA at latitude 38 degrees 37 minutes and 44 seconds.

(20)

3.1.2 Stability in Water

Type: abiotic
t1/2 pH : > 100 day
Degradation: < 5 % after
Method: other: test conditions not documented
Year: 1983 **GLP:** no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles

(21)

3.1.3 Stability in Soil

Type: laboratory **Radiolabel:** no
Concentration: 117 mg/kg
Soil temp.: 20 degree C
Soil humidity: 25 other: %
Soil classif.: other: U.S.D.A. class silt loam **Year:** 1985
Content of clay: = 15 %
silt: = 63 %
sand: = 22 %
pH: = 7.2
Cation exch. capac. = .71 other: moles/100 g soil dry weight
Microbial biomass:
Dissipation time DT50: = 59.2 day
Dissipation: = 24 % after 135 day
Method: other: Biological soil reactor method
Year: 1985 **GLP:** no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles

(22)

Type: laboratory **Radiolabel:** no
Concentration: 500 mg/kg
Soil temp.: 60 degree C
Cation exch. capac.
Microbial biomass:
Dissipation time Dissipation: = 75 % after 7 day
Method: other: Degradation in compost
Year: 1982 **GLP:** no data
Test substance: other TS: Purchased from Chem Service
Source: Monsanto Europe N.V. Bruxelles

(23)

3.2 Monitoring Data (Environment)

Type of measurement: background concentration
Medium: sediment
Remark: 9 of 122 samples had BBP; geometric mean <.2 over 3 years
Source: Monsanto Europe N.V. Bruxelles
(24)

Type of measurement: background concentration
Medium: surface water
Remark: 15 of 204 samples had BBP; geometric mean <.5 over 3 years
Source: Monsanto Europe N.V. Bruxelles
(25)

Type of measurement: background concentration
Medium: drinking water
Remark: 38 mg/l found in New York; EPA's Council on Environmental Quality Survey
Source: Monsanto Europe N.V. Bruxelles
(26)

Type of measurement: background concentration
Medium: surface water
Remark: 12 day study of Rhine river and Lake Yssel; for Rhine river water=.01ug/l, suspended particulate matter=.01 mg/kg; for Lake Yssel water<.01 ug/l, suspended particulate matter <.01 to .05 mg/kg
Source: Monsanto Europe N.V. Bruxelles
(27)

Type of measurement: background concentration
Medium: other: urban runoff water
Remark: 86 samples collected in US; 1% frequency of detection at 10 ug/l
Source: Monsanto Europe N.V. Bruxelles
(28)

Type of measurement: background concentration
Medium: drinking water
Remark: 39 wells tested; 5 well positive (13%); maximum detected level=38 ug/l
Source: Monsanto Europe N.V. Bruxelles
(29)

Type of measurement: background concentration
Medium: surface water
Remark: Delaware river water; 11 grab samples; conc. in winter=.4-1 ug/l (detected in only 5 samples; conc. in summer=.3 ug/l (detected in all 11 samples)
Source: Monsanto Europe N.V. Bruxelles
(30)

Type of measurement: background concentration
Medium: surface water
Remark: detected in lakes Ontario and Erie; SUMMARY PAPER
Source: Monsanto Europe N.V. Bruxelles
(31)

Type of measurement: background concentration
Medium: surface water
Remark: In Lake Michigan 2-4 ug/l in 2 of 13 sited tested; in Delaware river .4-1 ug/l in winter and .3 ug/l in summer
Source: Monsanto Europe N.V. Bruxelles
(32)

Type of measurement: background concentration
Medium: surface water
Remark: found 1 ug/l in Lake Michigan
Source: Monsanto Europe N.V. Bruxelles
(33)

Type of measurement: background concentration
Medium: surface water
Remark: avg approx. .35 ug/l
Source: Monsanto Europe N.V. Bruxelles
(34)

Type of measurement: background concentration
Medium: sediment
Remark: residue in sediments average 136 ng/g
Source: Monsanto Europe N.V. Bruxelles
(35)

Type of measurement: background concentration
Medium: sediment
Remark: 3 samples/location; 11 locations; found <100 ng/g to 567 ng/g; 25% of samples contained BBP
Source: Monsanto Europe N.V. Bruxelles
(36)

Type of measurement: background concentration
Medium: surface water
Remark: 3-5 samples/location; 11 locations; found 0.2 to 2.4 ug/l; 66% of samples contained BBP
Source: Monsanto Europe N.V. Bruxelles
(36)

Type of measurement: background concentration
Medium: biota
Remark: measured conc. in oysters; below detection limits (<.15 mg/l)
Source: Monsanto Europe N.V. Bruxelles
(37)

Type of measurement: background concentration
Medium: biota
Remark: 182 samples; mean conc.<2.5 ug/kg; numbers stored in STORET database
Source: Monsanto Europe N.V. Bruxelles
(38)

Type of measurement: background concentration
Medium: sediment
Remark: 392 samples; mean conc.<500 ug/kg; numbers stored in STORET database
Source: Monsanto Europe N.V. Bruxelles
(38)

Type of measurement: background concentration
Medium: surface water
Remark: 1220 samples; mean conc.<10 ug/l; numbers stored in STORET database
Source: Monsanto Europe N.V. Bruxelles
(38)

Type of measurement: background concentration
Medium: other: effluent
Remark: 1337 samples; mean conc.<6 ug/l; numbers stored in STORET database
Source: Monsanto Europe N.V. Bruxelles
(38)

Type of measurement: background concentration
Medium: surface water
Source: Monsanto Europe N.V. Bruxelles
(39)

Type of measurement: concentration at contaminated site
Medium: ground water
Remark: compound not detected, sampled well by landfill
Source: Monsanto Europe N.V. Bruxelles

(40)

Type of measurement: other: 3 municipal sludges
Medium: other: sludge
Remark: BBP=0.004% of oven dry wt. in 1 sludge; not detected in other 2 sludges.
Source: Monsanto Europe N.V. Bruxelles

(41)

Type of measurement: other: monitor effluent from sludge plant
Medium: other: effluent
Remark: influent sewage=8.0 ug/l; treated effluent=1.3 ug/l; aeration lagoon=1/0 ug/l
Source: Monsanto Europe N.V. Bruxelles

(36)

Type of measurement: other: monitoring poultry plant
Medium: other: processing water at poultry plant
Remark: grab sample on 4 different dates; compound tentatively identified, but not confirmed
Source: Monsanto Europe N.V. Bruxelles

(42)

Type of measurement: other: monitoring water plants
Medium: drinking water
Remark: sampled at 3 different plants; mean of 3 reps.; samples collected over 7 day period; Conc. range=.64-.83 ug/l
Source: Monsanto Europe N.V. Bruxelles

(43)

Type of measurement: other: treated effluent
Medium: other: effluent
Remark: influent 40 ug/l; effluent 100 ug/l; final discharge in drinking water 0.4 ug/l
Source: Monsanto Europe N.V. Bruxelles

(44)

3.3.1 Transport between Environmental Compartments

Type: adsorption
Media: water - soil
Method: other: Fed. Reg. 44:16240-92.
Year: 1979
Remark: measured soil adsorption coefficient=68-350
Source: Monsanto Europe N.V. Bruxelles
Test condition: 3 soils with organic matter ranging from 1.2-3.4%; initial conc. in water ranged from 0-1 mg/l; mixture shaken 24hrs then aqueous solution analyzed; 20C

(36)

Type: volatility
Media: water - air
Method: other: test conditions undocumented
Year: 1980
Remark: at 200C volatility is high
Source: Monsanto Europe N.V. Bruxelles

(36)

3.3.2 Distribution

-

3.4 Mode of Degradation in Actual Use

-

3.5 Biodegradation

Type: aerobic
Inoculum: predominantly domestic sewage
Concentration: 100 mg/l
Degradation: = 88 % after 28 day
Method: Directive 84/449/EEC, C.7 "Biotic degradation - modified MITI test"
Year: 1989 **GLP:** no
Test substance:
Remark: MEETS 10 DAY WINDOW
Data related to O2 consumption
Source: Monsanto Europe N.V. Bruxelles

(45)

Type: aerobic
Inoculum: activated sludge, adapted
Concentration: 20 mg/l related to Test substance
Degradation: = 93 % after 28 day
Result: readily biodegradable
Kinetic:
1 day = 6 %
2 day = 29 %
3 day = 46 %
4 day = 58 %
6 day = 69 %
Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year: 1981 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(46)

Type: aerobic
Inoculum: activated sludge, adapted
Concentration: 20 mg/l related to Test substance
Degradation: = 96 % after 27 day
Result: readily biodegradable
Kinetic:
1 day = 5 %
2 day = 27 %
3 day = 45 %
4 day = 58 %
6 day = 68 %
Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year: 1981 **GLP:** no data
Test substance: no data
Remark: Study referenced method of Thompson-Duthie-Sturm (1973), Journal of American Oil Chemists' Society 50, 159. Values listed in kinetic section are estimated from graphed data. Results are in %CO2 evolved.
Source: Monsanto Europe N.V. Bruxelles

(47)

Type: aerobic
Inoculum: activated sludge
Concentration: 133 mg/l related to Test substance
Degradation: > 99 % after 24 hour(s)
Result: other: % removal measured as primary biodegradation; also obtained 93%primary removal at a dose of 3 mg/l
Method: OECD Guide-line 302 A "Inherent Biodegradability: Modified SCAS Test"
Year: 1981 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(48)

Type: aerobic
Inoculum: activated sludge, adapted
Concentration: 200 mg/l related to Test substance
Degradation: > 99 % after 24 hour(s)
Result: other: % primary biodegradation removal; also observed 93% primaryremoval in 24 hours at a dose of 5 mg/l
Method: OECD Guide-line 302 A "Inherent Biodegradability: Modified SCAS Test"
Year: 1981 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Biodegradation of half-ester, monobutyl phthalate, was determined in SCAS test. Half-life in SCAS was found to be less than 0.1 days once organisms were acclimated. Formation of biodegradation intermediates followed as benzyl butyl phthalate biodegraded. Intermediates were biodegraded to the extent that they were at detection limit in 14 hours after initial dose with benzyl butyl phthalate.
Source: Monsanto Europe N.V. Bruxelles

(46)

Type: aerobic
Inoculum: activated sludge
Concentration: .013 mg/l related to Test substance
Degradation: = 100 %
Result: other: removal from activated sludge aeration basin
Method: other
Year: **GLP:** no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles

(49)

Type: aerobic
Inoculum: domestic sewage
Concentration: 10 mg/l related to Test substance
Degradation: = 100 % after 7 day
Result: other: Primary biodegradation measured. Complete in less than 7 days.
Kinetic:
7 day = 100 %
14 day = 100 %
21 day = 100 %
28 day = 100 %
Method: other: Bunch and Chambers (1967), Journal of the Water Pollution ControlFederation 39, 181.
Year: 1967 **GLP:** no data
Test substance: no data
Remark: Significant biodegradation with rapid acclimation was observed.
Source: Monsanto Europe N.V. Bruxelles

(50)

Type: aerobic
Inoculum: activated sludge
Concentration: 20 mg/l related to Test substance
Degradation: = 43 - 88 % after 28 day
Result: other: Acclimation period appears to be variable.
Kinetic:

3 day	= 1 - 2 %
7 day	= 4 - 8 %
9 day	= 4 - 12 %
14 day	= 6 - 42 %
21 day	= 18 - 71 %

Method: other: CO2 evolution method similar to U.S. EPA TSCA method 40 CFR Ch 1subpart D paragraph 796.3100.
Year: 1992 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Primary degradation after 28 days: 77.7 - >97%
Source: Monsanto Europe N.V. Bruxelles

(51)

Type: aerobic
Inoculum: other: Mycobacterium sp. and Nocardia sp.
Concentration: 20 mg/l related to Test substance
Result: other: Mycobacterium and Nocardia sp. could use benzyl butyl phthalateas sole carbon source for growth.
Method: other: Gibbons and Alexander protocol; see test conditions
Year: 1989 **GLP:** no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
Test condition: Replication in broth.

(52)

Type: aerobic
Inoculum: other: lake water microcosm
Concentration: 1 mg/l related to Test substance
Degradation: = 99.8 % after 14 day
Result: other: Half-life estimated to be approximately 1.5 days. Noconcentration dependence on biodegradation from 0.01 mg/l to 1 mg/l.Presence of sediment does not effect transformation rate.
Kinetic:

3 day	= 79 - 91 %
7 day	= 99 - 99 %
10 day	= 99 - 100 %
14 day	= 100 - 100 %

Method: other: Method of Bourquin, A.W. et al.(1977), Developmental & IndustrialMicrobiology 18,185-191.
Year: 1977 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Test substance: Two samples of benzyl butyl phthalate were prepared. One ring labeled and the other carbonyl labeled. The ring labeled material had a 97% radiochemical purity.

(53)

Type: aerobic
Inoculum: domestic sewage
Concentration: 5 mg/l related to Test substance
Degradation: > 90 % after 7 day
Result: other: Greater than 90% primary biodegradation observed.
Method: other: Patterson and Kodukala protocol; see test conditions
Year: 1981 **GLP:** no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
Test condition: Shake-flask test.

(54)

Type: aerobic
Inoculum: activated sludge
Concentration: 33.5 mg/l related to Test substance
Degradation: > 96 %
Result: other: In model sewage treatment >96% removal from effluent. Removalattributed to absorption in primary.
Method: other: Petrasek et al. protocol; see test conditions
Year: 1983 **GLP:** no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
Test condition: Model sewage treatment.

(55)

Type: aerobic
Inoculum:
Concentration: 3.3 mg/l
Degradation: = 93 % after 1 day
Method: other: SCAS test
Year: **GLP:**
Test substance:
Source: Monsanto Europe N.V. Bruxelles

(56)

Type: aerobic
Inoculum: other: selected specific microorganisms
Concentration: 500 mg/l related to Test substance
Result: other: identified organisms capable of using benzyl butyl phthalate as agrowth medium. These organisms are found in river water, river sedimentand in estuaries.
Method: other: Taylor et al. protocol; see test conditions.
Year: 1981 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Test condition: Difco laboratories solid media.
Test substance: Test substance supplied by Monsanto.

(57)

Type: aerobic
Inoculum: other: microcosm study, sediment and water obtained from IllinoisRiver near Pere Marquette State Park which is 3 miles north of Grafton,Illinois.
Concentration: .1 mg/l related to Test substance
Degradation: = 50 % after 2.2 day
Result: other: half-life estimated to be 2.2 days at a dose of 0.1 mg/l and 1.5days at a dose of 0.01 mg/l. Half-life became shorter as microorganismsbecame acclimated.
Method: other: U.S.E.P.A. (1983) Experimental marine microcosm test protocol andsupport document: measurement of the ecological effects, fate andtransport of chemicals in site-specific marine ecosystems. EPA Ecol.Research Series #60013-83-055
Year: 1983 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Test substance: Santicizer 160 (benzyl butyl phthalate) purity used for this study was 98.6% Lot # DD243. The radiolabeled benzyl butyl phthalate used in this study had a purity greater than 94.4%.

(58)

Type: aerobic
Inoculum: activated sludge
Concentration: 100 mg/l
Degradation: = 81 % after 14
Method: other: see remarks
Year: **GLP:**
Test substance:
Remark: Method:
Biodegradation test of chemical substance by micororganisms etc. stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "301C, Ready Biodegradability: Modified MITI Test I" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981) related to BOD;

Sludge conc: 30 mg/l
Source: Monsanto Europe N.V. Bruxelles

(59)

Type: aerobic
Inoculum: activated sludge
Degradation: = 99 % after 48 hour(s)
Method: other: see test conditions
Year: 1973 **GLP:** no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
Test condition: SCAS test.

(60)

Type: aerobic
Inoculum: activated sludge, adapted
Concentration: .1044 mg/l related to Test substance
Degradation: > 95 % after 5 day
Result: other: primary biodegradation, <0.005 mg/l detected after 5 days.
Method: other: see test conditions
Year: 1978 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Test condition: River die-away at ambient temp; initial dose 0.1044 mg/L.

(61)

Type: aerobic
Inoculum: other: Mississippi River water at St. Louis MO USA after settling.
Concentration: 1 mg/l related to Test substance
Degradation: > 99 % after 14 day
Result: other: Primary biodegradation monitored.
Kinetic:

0 day	= 14.1 %
2 day	= 81.4 %
5 day	= 97.9 %
7 day	= 98.4 %
14 day	> 99 %

Method: other: see test conditions
Year: 1981 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Test condition: River die-away test at ambient temperature.

(46)

Type: aerobic
Inoculum: other: Settled Mississippi river water from St.Louis, MO USA
Concentration: .5 mg/l related to Test substance
Degradation: > 99 % after 2 day
Result: other: River-die-away greater than 99% primary biodegradation
Kinetic:

1 day	= 26.4 - 32.8 %
2 day	> 99 %

Method: other: see test conditions
Year: 1982 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Also evaluated rate of removal of 0.05 mg/l dosed river water. Observed average of 0.013 mg/l after 1 day and less than 0.005 mg/l after 2 days. Sterile control dosed at 0.5 mg/l had 0.449 mg/l remaining after 5 days.
Source: Monsanto Europe N.V. Bruxelles
Test condition: River die-away test at ambient temperatures.

(62)

Type: aerobic
Inoculum: other: settled river water from St. Louis USA area.
Concentration: 1 mg/l related to Test substance
Degradation: = 50 % after 2 day
Result: other: Time for 50% primary biodegradation in river-water determined.
Method: other: see test conditions
Year: 1975 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Test condition: River die-away test at ambient temperatures.

(63)

Type: aerobic
Inoculum:
Degradation: = 87.5 %
Method: other: shake flask method
Year: **GLP:**
Test substance:
Remark: related to CO2 production
Source: Monsanto Europe N.V. Bruxelles

(64)

Type: aerobic
Inoculum: activated sludge
Concentration: 3.3 mg/l
Degradation: = 99 % after 2 day
Method:
Year: **GLP:**
Test substance:
Source: Monsanto Europe N.V. Bruxelles

(65)

Type: anaerobic
Inoculum: anaerobic sludge
Concentration: .8 mmol/l related to Test substance
Degradation: = 0 - 24 % after 28 day
Result: other: Anaerobic biodegradation observed in 10% sludge dosed samplesfrom Jackson wastewater treatment facility but not from Adrian sludge.
Method: other: Horowitz et al. protocol; see test conditions
Year: 1982 **GLP:** no data
Test substance: other TS: >95% purity
Source: Monsanto Europe N.V. Bruxelles
Test condition: Formation of methane and CO2 from samples incubated with 10% digester sludge was monitored.

(66)

Type: anaerobic
Inoculum: anaerobic sludge
Concentration: 10 mg/l related to Test substance
Degradation: > 90 % after 8 day
Result: other: Benzyl butyl phthalate is anaerobically biodegradable in theconcentration ranges tested from 0.5 mg/l to 10 mg/l.
Kinetic: 107 hour(s) = 50 %
Method: other: Method similar to that described by Fedorak and Hrudley (1984).
Year: **GLP:** no data
Test substance: other TS: Chem Service
Source: Monsanto Europe N.V. Bruxelles

(67)

Type: anaerobic
Inoculum: anaerobic sludge
Concentration: .2 mmol/l related to Test substance
Degradation: = 97 % after 36 day
Result: other: Data indicates that benzyl butyl phthalate is anaerobicallybiodegradable.
Kinetic: 22 day = 78 %
36 day = 97 %
Method: other: Method similar to that described by Huntgate and by Balch et al.
Year: **GLP:** no data
Test substance: other TS: Purchased from Chem Service
Source: Monsanto Europe N.V. Bruxelles

(68)

Type: anaerobic
Inoculum: anaerobic sludge
Concentration: 20 mg/l related to Test substance
Degradation: = 100 % after 50 day
Result: other: Anaerobically biodegradable. Reached 100% of theoreticalmethane production.
Kinetic: 7 day = 60 %
14 day = 75 %
21 day = 85 %
28 day = 95 %
35 day = 97 %
Method: other: Shelton et al. protocol; see test conditions.
Year: 1984 **GLP:** no data
Test substance: other TS: Radiolabeled material provided by Monsanto.
Source: Monsanto Europe N.V. Bruxelles
Test condition: Anaerobic biodegradation of radiolabeled benzyl butyl phthalate was monitored in primary sludge from Jackson, Mississippi sewage treatment facility.

(69)

Type: anaerobic
Inoculum:
Degradation: < 10 % after 28 day
Result: under test conditions no biodegradation observed
Method: other: test conditions undocumented.
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(36)

Type: anaerobic
Inoculum:
Degradation: > 90 % after 40 day
Method:
Year: **GLP:**
Test substance:
Source: Monsanto Europe N.V. Bruxelles

(70)

3.6 BOD5, COD or BOD5/COD Ratio

-

3.7 Bioaccumulation

Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 17 day at 22 degree C
Concentration: .00222 mg/l
BCF: = 187.65
Elimination: no data
Method: other: ASTM Proposed Standards Practice for Conducting BioconcentrationTests with Fishes and Salt Water Bivalve Molluses. Draft 9.
Year: 1979 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: 14C; BCF listed for whole fish; T1/2 for whole fish=.91 day; For muscle BCF=28.54 and T1/2=1.14 day; For viscera BCF=1693.25 and T1/2= .67 day; For whole fish rate of uptake=143 and clearance=.75
Source: Monsanto Europe N.V. Bruxelles

(71)

Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 3 day at 22 degree C
Concentration: .034 mg/l
BCF: = 12
Elimination: no data
Method: other: EPA. Environmental Effects Test Guidelines. EPA 560/6-82-002
Year: 1982 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: BCF DETERMINED FOR PARENT COMPOUND ALONE; 14C; BCF listed for whole fish; conc. in whole fish=.415 mg/kg; for viscera BCF=19 and conc.=.653 mg/kg; for fillet BCF=1 and conc.=.038 mg/kg
Source: Monsanto Europe N.V. Bruxelles

(72)

Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 21 day at 16 degree C
Concentration: 9.73 µg/l
BCF: = 663
Elimination: yes
Method: other: Monsanto protocol; see test conditions
Year: 1980 **GLP:** no data
Test substance: no data
Remark: BCF DETERMINED FOR PARENT COMPOUND AND METABOLITES, FOR PARENT ALONE BCF=12 (SEE MONSANTO REPORT M0-92-9760); 7 day depuration; half life in tissue >1<2 days
Source: Monsanto Europe N.V. Bruxelles
Test condition: continual-flow "closed" system; 14C

(73)

3.8 Additional Remarks

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AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: flow through
Species: Parophrys vetulus (Fish, marine)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: = .55
Method: other: ASTM E729-80. Standard Guide for Conducting Acute Toxicity Testswith Fishes, Macroinvertebrates & Amphibians
Year: 1980 **GLP:** no data
Test substance: no data
Remark: C.I.=.48-.64 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: 20 L chambers; 10 L volume exchange/day; 140 ml/min flow rate; seawater

(74)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 14 day
Unit: mg/l **Analytical monitoring:** yes
LC50: = 2.25
Method: OECD Guide-line 204 "Fish, Prolonged Toxicity Test: 14-day Study"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(75)

Type: semistatic
Species: Parophrys vetulus (Fish, marine)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: = .66
Method: other: ASTM E729-80. Standard Guide for Conducting Acute Toxicity Testswith Fishes, Macroinvertebrates & Amphibians
Year: 1980 **GLP:** no data
Test substance: no data
Remark: C.I.=.53-.84 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: temp=12C; 16 hr light; 80% renewal/day; seawater

(74)

Type: static
Species: Cyprinodon variegatus (Fish, estuary, marine)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: > 2.69
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: TOXICITY ABOVE LEVEL OF WATER SOLUBILITY (2.69 MG/L); 96hr LC50=3 mg/l; 24hr LC50=approx. 7.5 mg/l; 48hr LC50=3.2 mg/L
Source: Monsanto Europe N.V. Bruxelles

(76)

Type: static
Species: Cyprinus auratus
Exposure period:
Unit: mg/l **Analytical monitoring:** no
LC50: > 2.69
Method: other: unknown
Year: 1975 **GLP:** no data
Test substance: other TS: 1.5% di-n-butylphthalate; .3% of other similar ester
Remark: TOXCITY ABOVE LEVEL OF WATER SOLUBILITY (2.69 mg/l); LC50 ca. 200 mg/l; resting heart rate ca. 105 beats/min; at 100 mg/l mean heart rate=105 beats/min; at 200 mg/l mean heart rate=40 beats/min
Source: Monsanto Europe N.V. Bruxelles

(77)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = .36
LC50: = 1.7
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: 24hr LC50=3.6 mg/l; 48 and 72hr LC50=1.7 mg/l
Source: Monsanto Europe N.V. Bruxelles

(78)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: > 2.69
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 **GLP:** no data
Test substance: no data
Remark: TOXICITY ABOVE LEVEL OF WATER SOLUBILITY (2.69 mg/l); 96hr LC50=43 mg/l (C.I.=38-52 mg/l); 24hr LC50=62 mg/l
Source: Monsanto Europe N.V. Bruxelles

(79)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: 1 - 10
Method: other: test conditions undocumented
Year: 1974 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: 96hr EC50=1.0 mg/l. Unacceptable study, undocumented data.
Source: Monsanto Europe N.V. Bruxelles

(80)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: < .36
LC50: > 2.69
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: TOXICITY ABOVE LEVEL OF WATER SOLUBILITY (2.69 mg/l); 96hr LC50=3.3 mg/l; 24hr LC50=4.8 mg/l; 48 and 72hr LC50=3.3 mg/l
Source: Monsanto Europe N.V. Bruxelles

(81)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: 1 - 10
Method: other: test conditions undocumented
Year: 1974 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: 96hr EC50=1.0 mg/l. Unacceptable study, undocumented data.
Source: Monsanto Europe N.V. Bruxelles

(80)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = 1
LC50: = 2.1
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: 24hr LC50=3.3 mg/l; 48hr LC50=2.1 mg/l; 72hr LC50=2.1 mg/l
Source: Monsanto Europe N.V. Bruxelles

(82)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = 2.2
LC50: > 2.69
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: TOXICITY ABOVE LEVEL OF WATER SOLUBILITY 92.69 mg/l); 96hr LC50 5.3 mg/l; 24hr LC50=10 mg/l; 48hr LC50=5.3 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: test conducted in hard water

(83)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = .57
EC50: = .97
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance: other TS: as prescribed by 1.1-1.4 but with 1:1 mixture with Di-2-EthyhexylPhthalate Esters
Remark: 24hr EC50>4.2 mg/l
48hr EC50 of BBP alone = 3.7 mg/l; of DEHP along = 2.0 mg/l
Source: Monsanto Europe N.V. Bruxelles

(84)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = .62
EC50: = 1.6
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** no data
Test substance: no data
Remark: When tests conducted in presence of food (2 mg/l algae or 30 mg/l YTCF) EC50>10 mg/l and NOEC<1.25 mg/l
Source: Monsanto Europe N.V. Bruxelles

(85)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: = 1.7
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: 168hr aged EC50=4.8 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: spiked test solution left to sit 168 hours before starting second tox test

(86)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = 1.8
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles

(87)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = .82
EC50: = 1.83
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** no data
Test substance: other TS
Remark: 24hr EC50=3.76 mg/l; Also looked at toxicity of metabolites: phthalic acid 48hr EC50>640 mg/l and NOEC>640 mg/l; Monobutyl 48hr EC50>320 mg/l and NOEC=160 mg/l; Monobenzyl 48hr EC50>160 mg/l and NOEC=40 mg/l
Source: Monsanto Europe N.V. Bruxelles

(88)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = 1
EC50: = 1.91
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance: other TS: as prescribed by 1.1-1.4 with 250 ppm fulvic acid
Remark: Fulvic acid could combine with alkyl phthalates to form soluble conplexes; without fulvic acid 48hr EC50=3.7 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: fulvic acid added at 250 ppm

(89)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = 1
EC50: > 2.69
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: TOXICITY ABOVE LEVEL OF WATER SOLUBILITY (2.69 mg/l); 48hr EC50=3.7 mg/l (C.I.=3-4.6); 24hr EC50=7.2 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: lake water; temp=23C; hardness=110 mg/l CaCO3

(90)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
NOEC: = 1
EC50: > 2.69
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TOXICITY ABOVE LEVEL OF WATER SOLUBILITY (2.69 mg/l); 48hr EC50=4.8 mg/l (C.I.=2.4-9.6 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: test solution aged 168 hours before starting the test; no biodegradation noted

(91)

Species: Mysidopsis bahia (Crustacea)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = .4
EC50: = .9
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: 24hr EC50>3 mg/l; 48hr EC50=2.2 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: temp=20C; salinity=18 g/l; natural seawater

(92)

Species: Mysidopsis bahia (Crustacea)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
NOEC: = .12
EC50: = .74
Method: other: Federal Register. Mysid Shrimp Acute Toxicity Test
Year: 1985 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: solubility in seawater is approx. 1.0 mg/l; 96hr EC50 is 0.74;
Source: Monsanto Europe N.V. Bruxelles
Test condition: highest tested conc. = .74 mg/l(measured); 20 organisms per treatment; flow through system

(93)

Species: other: Chironomus tentans
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = 1.6
Method: other: ASTM. Standard Guide for Conducting Acute Toxicity Tests withFishes, Macroinvertebrates and Amphibians. ASTM E729-80.
Year: 1980 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Test condition: 40 ml test solution; 10 reps; 1 organism per chamber; temp=22C; well water

(87)

Species: other: Chironomus tentans
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = 1.25
EC50: = 1.64
Method: other: EPA. Methods for Acute Toxcity Tests with Fish,Macroinvertebrates, and Amphibians. EPA-660/3-75-009
Year: 1975 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: 24hr EC50=2.69 mg/l
Source: Monsanto Europe N.V. Bruxelles

(94)

Species: other: Chironomus tentans
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: > 2.69
Method: other: Springborn Laboratory protocol; see test conditions
Year: 1981 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TOXICITY ABOVEL LEVEL OF WATER SOLUBILITY (2.69 mg/l); 48hr LC50=3.6 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: carrier-acetone; 200 ml test solution; 5 larvae/beaker; pH=7.6; temp=22C

(95)

Species: other: Paratanytarsus dissimilis
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: > 2.69
Method: other: Springborn Laboratories protocol; see test conditions
Year: 1981 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TOXICITY ABOVE LEVEL OF WATER SOLUBILITY (2.69 mg/l); 48hr LC50=3.6 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: carrier-acetone; 200 ml test solution; 5 larvae/beaker; pH=7.6; temp=22C

(95)

Species: other: Paratanytarus parthenogenetica
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: > 2.69
EC50: > 2.69
Method: other: EPA. Methods for Acute Toxicity Tests with Fish,Macroinvertebrates and Amphibians, EPA-660/3-75-009
Year: 1975 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: TOXICITY ABOVE LEVEL OF WATER SOLUBILITY (2.69 mg/l); 48hr EC50=7.2 mg/l; 24hr EC50>8 mg/l; 48hr NOEC=4 mg/l
Source: Monsanto Europe N.V. Bruxelles

(96)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Dunaliella tertiolecta (Algae)
Endpoint: other: in vivo chlorophyll
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = .3
EC50: = 2
Method: other: Manual of Analytical methods for the Analysis of PesticideResidues in Human and Environmental Samples
Year: 1978 **GLP:** yes
Test substance: other TS
Remark: TESTS WERE CARRIED OUT WITH TEST MATERIAL THAT IS NO LONGER REPRESENTATIVE OF CURRENT PRODUCTION USING SOLVENTS TO ENHANCE SOLUBILITY AND THEREFORE SHULD NOT BE USED FOR CLASSIFICATION. ADDITIONAL STUDIES WITH CURRENT TEST MATERIAL ARE IN PROGRESS;

GOOD CORRELATION HAS BEEN ESTABLISHED BETWEEN IN VIVO CHLOROPHYLL A VALUE AND CELL COUNT NUMBER (Environmental Assessment Technical Assistance Document 4.01--Algal Assay prepared by the Environmental Staffs of the Center for Food Safety and Applied Nutrition and the Center for Veterinary Medicine, 1987);

other in vivo chlorophyll results - 24hr EC50>3 mg/l, 48hr EC50>3 mg/l, 96hr EC50=1 mg/l; 96hr EC50 based on cell count=1 mg/l

Source: Monsanto Europe N.V. Bruxelles
Test condition: carrier-acetone; 30 ppt salinity; temp=20C; 2000 lux

(97)

Species: Microcystis aeruginosa (Algae, blue, cyanobacteria)
Endpoint: biomass
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: > 2.69
EC50: > 2.69
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 **GLP:** yes
Test substance: other TS
Remark: TESTS WERE CARRIED OUT WITH TEST MATERIAL THAT IS NO LONGER REPRESENTATIVE OF CURRENT PRODUCTION USING SOLVENTS TO ENHANCE SOLUBILITY AND THEREFORE SHOULD NOT BE USED FOR CLASSIFICATION. ADDITIONAL STUDIES WITH CURRENT TEST MATERIAL ARE IN PROGRESS;

TOXICITY ABOVE LEVEL OF WATER SOLUBILITY (2.69 mg/l); 96hr EC50=1000 mg/l; 96hr NOEC=560 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: init. inoc=50000 cells/ml; 4000 lux; temp=24C; Algal Assay Media

(98)

Species: Navicula pelliculosa (Algae)
Endpoint: other: in vivo chlorophyll
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = .3
EC50: = .9
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 **GLP:** yes
Test substance: other TS
Remark: TESTS WERE CARRIED OUT WITH TEST MATERIAL THAT IS NO LONGER REPRESENTATIVE OF CURRENT PRODUCTION USING SOLVENTS TO ENHANCE SOLUBILITY AND THEREFORE SHOULD NOT BE USED FOR CLASSIFICATION. ADDITIONAL STUDIES WITH CURRENT TEST MATERIAL ARE IN PROGRESS;

GOOD CORRELATION HAS BEEN ESTABLISHED BETWEEN IN VIVO CHLOROPHYLL A VALUE AND CELL COUNT NUMBER (Environmental Assessment Technical Assistance Document 4.01--Algal Assay prepared by the Environmental Staffs of the Center for Food Safety and Applied Nutrition and the Center for Veterinary Medicine, 1987);

other in vivo chlorophyll results - 24hr EC50=2 mg/l, 48hr EC50=1 mg/l, 96hr EC50=.6 mg/l; 96hr EC50 based on cell count=.6 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: temp=24C; 4000 lux; Algal Assay Media

(99)

Species: Selenastrum capricornutum (Algae)
Endpoint: biomass
Exposure period: 14 day
Unit: mg/l **Analytical monitoring:** yes
NOEC: < .02
EC50: = .52
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 **GLP:** no data
Test substance: other TS
Remark: TESTS WERE CARRIED OUT WITH TEST MATERIAL THAT IS NO LONGER REPRESENTATIVE OF CURRENT PRODUCTION USING SOLVENTS TO ENHANCE SOLUBILITY AND THEREFORE SHOULD NOT BE USED FOR CLASSIFICATION. ADDITIONAL STUDIES WITH CURRENT TEST MATERIAL ARE IN PROGRESS;

5 day EC50=.72 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: temp=24C; 4000 lumens; "cool" white lights; Algal Assay Media

(100)

Species: Selenastrum capricornutum (Algae)
Endpoint: biomass
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = .52
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 **GLP:** no data
Test substance: other TS
Remark: TESTS WERE CARRIED OUT WITH TEST MATERIAL THAT IS NO LONGER REPRTSENTATIVE OF CURRENT PRODUCTION USING SOLVENTS TO ENHANCE SOLUBILITY AND THEREFORE SHOULD NOT BE USED FOR CLASSIFICATION; ADDITIONAL STUDIES WITH CURRENT TEST MATERIAL ARE IN PROGRESS; 96hr EC10=.21 mg/l; 96hr EC90=.83 mg/l
Source: Monsanto Europe N.V. Bruxelles

(101)

Species: Selenastrum capricornutum (Algae)
Endpoint: other: in vivo chlorophyll
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = .1
EC50: = .7
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 **GLP:** yes
Test substance: other TS
Remark: TESTS WERE CARRIED OUT WITH TEST MATERIAL THAT IS NO LONGER REPRESENTATIVE OF CURRENT PRODUCTION USING SOLVENTS TO ENHANCE SOLUBILITY AND THERFORE SHOULD NOT BY USED FOR CLASSIFICATION. ADDITIONAL STUDIES WITH CURRENT TEST MATERIAL ARE IN PROGRESS;

GOOD CORELATION HAS BEEN ESTABLISHED BETWEEN IN VIVO CHLOROPHYLL A VALUE AND CELL COUNT NUMBER (Environmental Assessment Technical Assistance Document 4.01--Algal Assay prepared by the Environmental Staffs of the Center for Food Safety and Applied Nutrition and the Center for Veterinary Medicine, 1987);

other in vivo chlorophyll results - 24hr EC50>3 mg/l, 48hr EC50=1 mg/l, 96hr EC50=.5 mg/l; 96hr EC50 based on cell counts=.4 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: temp=24C; 4000 lux; init. inoc.=10000 cells/ml; Algal Assay Media; "cool" white lights

(102)

Species: Skeletonema costatum (Algae)
Endpoint: other: in vivo chlorophyll
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = .5
Method: other: Manual of Analytical Methods for the Analysis of PesticideResidues in Human and Envoronmental Samples, 1974, Pesticides and ToxicSubstances Effects Laboratory National Environ. Res. Cent., Res. TrianglePark, NC Sect. 5A(4),(a)
Year: 1978 **GLP:** yes
Test substance: other TS
Remark: GOOD CORRELATION HAS BEEN ESTABLISHED BETWEEN IN VIVO CHLOROPHYLL A VALUE AND CELL COUNT NUMBERS (Environmental Assessment Technical Assistance Document 4.01--Algal Assay prepared by the Environmental Staffs of the Center for Food Safety and Applied Nutrition and the Center for Veterinary Medicine, 1987); other in vivo chlorophyll results - 24hr EC50=.9 mg/l, 48hr EC50=.4 mg/l, 96hr EC50=.4 mg/l; 96hr EC50 based on cell count=.6 mg/l; MARINE ALGAE--THIS DATA DISREGARDED FOR LABELLING/CLASSIFICATION
Source: Monsanto Europe N.V. Bruxelles
Test condition: carrier-acetone; temp=20C; 30 ppt salinity; 20C; 2000 lux

(103)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 30 minute(s)
Unit: mg/l **Analytical monitoring:** no
EC50: < 2.9
Method: OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year: 1984 **GLP:** no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
Test condition: more dilute cell and substrate concentrations (75 mg/l and 375 mg/l); sealed vessels by polytetrafluoroethylene plug;; pH=6.7-7.3; temp=24-26C

(104)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: Pimephales promelas (Fish, fresh water)
Endpoint: other: hatching, growth
Exposure period: 30 day
Unit: mg/l **Analytical monitoring:** yes
NOEC: .14 - .36
MATC : = .22
Method: other: Benoit, D.A. et al protocol
Year: 1982 **GLP:** no data
Test substance: no data
Remark: hatching of enbryos, survival of larvae and growth of larvae was significantly reduced at 0.36 mg/l; analytical monitoring: GC/ECD
Source: Monsanto Europe N.V. Bruxelles

(105)

Species: Pimephales promelas (Fish, fresh water)
Endpoint: other: survival
Exposure period: 14 day
Unit: mg/l **Analytical monitoring:** yes
LOEC: = 1.06
Method: other: Gledhill, W.E. et al protocol
Year: 1980 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: LC50=2.25 mg/l
Source: Monsanto Europe N.V. Bruxelles

(106)

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Endpoint: reproduction rate
Exposure period: 21 day
Unit: mg/l **Analytical monitoring:** yes
NOEC: = .26
MTC : .26 - .76
Method: other: Monsanto protocol; see test conditions
Year: 1979 **GLP:** yes
Test substance: as prescribed by 1.1 - 1.4
Remark: max. tox. conc.; survival same up to 21 days; reproduction decreased at .76 mg/l at day 21
Source: Monsanto Europe N.V. Bruxelles
Test condition: continuously exposed; went through 2 generations; reconstituted water; Mount and Brungs diluter; 1.75L aquaria
(107)

Species: Daphnia magna (Crustacea)
Endpoint: reproduction rate
Exposure period: 21 day
Unit: mg/l **Analytical monitoring:** yes
MATC : .22 - .35
Method: other: Monsanto protocol; see test conditions
Year: 1983 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Max. Accept. Tox. Conc. based on 21 day growth: >0.35<0.70 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: renewal 3 times/week; well water; carrier-DMF
(108)

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

-

4.6.2 Toxicity to Terrestrial Plants

-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

-

4.7 Biological Effects Monitoring

-

4.8 Biotransformation and Kinetics

-

4.9 Additional Remarks

-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 2330 mg/kg bw
Method: Directive 84/449/EEC, B.1 "Acute toxicity (oral)"
Year: 1984 **GLP:** no
Test substance: other TS
Source: Monsanto Europe N.V. Bruxelles
Test substance: purity 97.2%

(109)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 20400 mg/kg bw
Method: other
Year: 1976 **GLP:** no
Test substance:
Source: Monsanto Europe N.V. Bruxelles

(110)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 4000 mg/kg bw
Method: other
Year: 1974 **GLP:** no
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles

(111)

Type: other
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: > 4000 mg/kg bw
Method: other: no data
Year: **GLP:** no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles

(112)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: = 4170 mg/kg bw
Method: Directive 84/449/EEC, B.1 "Acute toxicity (oral)"
Year: 1984 **GLP:** no data
Test substance: other TS
Source: Monsanto Europe N.V. Bruxelles
Test substance: purity 97.2%

(109)

Type: LD50
Species: other: no data
Sex:
Number of Animals:
Vehicle:
Value: = 13500 mg/kg bw
Method:
Year: **GLP:** no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles

(113)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: other: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 4 hour(s)
Value: > 6.7 mg/l
Method: other: Monsanto
Year: 1979 **GLP:** no
Test substance:
Source: Monsanto Europe N.V. Bruxelles

(114)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: > 10000 mg/kg bw
Method: other
Year: 1976 **GLP:** no
Test substance:
Remark: 10,000 mg/kg was a limit dose
Source: Monsanto Europe N.V. Bruxelles

(110)

Type: LD50
Species: other: no data
Sex:
Number of Animals:
Vehicle:
Value: = 6700 mg/kg bw
Method:
Year: **GLP:**
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles

(113)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: = 2656 mg/kg bw
Method: other
Year: **GLP:** no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles

(115)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: = 3160 mg/kg bw
Method: other
Year: **GLP:** no data
Test substance: other TS
Remark: Swis Webster mice
2510-3980 (95% confidence limit)
Source: Monsanto Europe N.V. Bruxelles
(116)

Type: other
Species: rat
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: > 1800 mg/kg bw
Method: other
Year: **GLP:** no data
Test substance: other TS
Remark: the animals died after 4-8 days; weight loss, apathy, leucocytosis; histological observations: toxic splenitis, degenerative lesions of the nervous system
Source: Monsanto Europe N.V. Bruxelles
(112)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.:
Method: Draize Test
Year: 1976 **GLP:** no
Test substance:
Remark: 0.5ml applied for 24 hrs to intact and abraded skin, 6 rabbits were tested
Source: Monsanto Europe N.V. Bruxelles
(117)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: moderately irritating
EC classificat.:
Method: other
Year: **GLP:** no data
Test substance: other TS
Remark: 2-4 rabbits tested in the patch test with undiluted test substance
Source: Monsanto Europe N.V. Bruxelles

(112)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: other
Year: **GLP:** no data
Test substance:
Remark: 15-30 volunteers;
10% solution (not specified)
No classification is assigned to this report because this is a poorly reported study that was conducted over 40 years ago.
Source: Monsanto Europe N.V. Bruxelles

(112)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.:
Method: Draize Test
Year: 1976 **GLP:** no
Test substance:
Remark: 6 rabbits tested;
0.1 ml of undiluted test material placed in eye
Source: Monsanto Europe N.V. Bruxelles

(110)

5.3 Sensitization

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method: other
Year: 1979 **GLP:** no
Test substance:
Remark: patches containing the undiluted material were applied to the skin of 200 subjects for 24 hours, 5 days a week for 3 weeks. Subjects were rechallenged at a virgin site after a 2 week rest period.
Source: Monsanto Europe N.V. Bruxelles

(118)

Type: no data
Species: human
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method: other
Year: 1952 **GLP:** no
Test substance:
Remark: 10% solution applied 2 weeks after primary irritation test 15-30 volunteers tested
Source: Monsanto Europe N.V. Bruxelles

(119)

5.4 Repeated Dose Toxicity

Species: rat **Sex:** male/female
Strain: Sprague-Dawley
Route of admin.: inhalation
Exposure period: 28 days
Frequency of treatment: 6h/day 5d/week
Post. obs. period: none
Doses: 0.36, 1.0, 2.0 mg/l (analytical concentration)
Control Group: yes
NOAEL: = 1 mg/l
Method: Directive 84/449/EEC, B.8 "Sub-acute toxicity (inhalation)"
Year: 1987 **GLP:** yes
Test substance:
Result: 1) 0.36 mg/l
no effects
2) 1.0 mg/l
NOEL
no effects
3) 2.1 mg/l
mortality;
body weight, decr;
spleen, atrophy;
testes, atrophy.
Source: Monsanto Europe N.V. Bruxelles

(120)

Species: rat **Sex:** male/female
Strain: Sprague-Dawley
Route of admin.: inhalation
Exposure period: 28 days
Frequency of treatment: 6 h/day 5d/week
Post. obs. period: none
Doses: .049, .144, .526 mg/l
Control Group: yes
NOAEL: = .144 mg/l
Method: other
Year: 1976 **GLP:** no
Test substance:
Remark: chamber concentrations were determined analytically
Result: 1) 0.049 mg/l
no effects
2) 0.144 mg/l
no effects
NOEL
3) 0.526 mg/l
body weight, decr;
Source: Monsanto Europe N.V. Bruxelles

(121)

Species: rat **Sex:** male/female
Strain: Sprague-Dawley
Route of admin.: inhalation
Exposure period: 90 days
Frequency of treatment: 6h/day 5days/wk
Post. obs. period: none
Doses: .051, .218, .789 mg/l
Control Group: yes
NOAEL: = .218 mg/l
Method: other
Year: 1979 **GLP:** yes
Test substance:
Result: 1) .051 mg/l:
no effects
2).218 mg/l:
NOEL
no effects
3).789 mg/l:
liver weight, incr;
kidney weight, incr.
Source: Monsanto Europe N.V. Bruxelles

(122)

Species: rat **Sex:** male/female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 28 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 500, 1000, 1500, 2000, 3000 mg/kg bw/day
Control Group: yes
NOAEL: = 1000 mg/kg bw
Method: other
Year: 1978 **GLP:** no
Test substance:
Result: 1) 500 mg/kg/day:
no effects
2) 1000 mg/kg/day:
NOEL
no effects
3) 1500 mg/kg/day:
body weight, decr.
4) 2000 mg/kg/day:
body weight, decr.
5) 3000 mg/kg/day:
bleeding around nares;
stiffness around hindlimbs when walking
Source: Monsanto Europe N.V. Bruxelles

(123)

Species: rat **Sex:** male/female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 28 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 500, 1000, 1500, 2000, 3000, 4000 mg/kg bw/day
Control Group: yes
NOAEL: = 1000 mg/kg bw
Method: other
Year: **GLP:** no
Test substance:
Result: 1) 500 mg/kg/day:
mo effects
2) 1000 mg/kg/day:
NOEL
no effects
3) 1500 mg/kg/day:
body weight, decr;
mortality.
4) 2000 mg/kg/day.
mortality;
body weight, decr;
hindlimbs, stiffness;
testes, atrophy;
5) 3000 mg/kg/day:
mortality;
body weight, decr;
hindlimbs, stiffness;
testes, atrophy.
6) 4000 mg/kg/day:
mortality;
body weight, decr;
hindlimbs, stiffness;
testes, atrophy.
Source: Monsanto Europe N.V. Bruxelles

(121)

Species: rat **Sex:** male/female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 42 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 500, 1500, 3000 mg/kg bw/d
Control Group: yes
NOAEL: = 500 mg/kg bw
Method: other
Year: **GLP:** no
Test substance:
Result: 1) 500 mg/kg/day:
NOEL
no effects
2) 1500 mg/kg/day:
body weight, decr.
3) 3000 mg/kg/day:
body weight, decr;
hindlimbs, transient stiffness while walking.
Source: Monsanto Europe N.V. Bruxelles

(121)

Species: rat **Sex:** male/female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 90 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 188, 375, 750, 1125, 1500 mg/kg bw/day
Control Group: yes
NOAEL: = 375 mg/kg bw
Method: other
Year: 1978 **GLP:** no
Test substance:
Result: 1) 188 mg/kg/day:
no effects
2) 375 mg/kg/day:
no effects
NOEL
3) 750 mg/kg/day:
kidney weight, incr.
4) 1125 mg/kg/day:
kidney weight, incr;
liver weight, incr.
5) 1500 mg/kg/day:
liver weight, incr;
kidney weight, incr.
Source: Monsanto Europe N.V. Bruxelles

(124)

Species: rat **Sex:** male/female
Strain: Wistar
Route of admin.: oral feed
Exposure period: 90 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 151, 381, 960 mg/kg bw/day (M)
Control Group: yes
NOAEL: = 151 mg/kg bw
Method: other
Year: 1978 **GLP:** no
Test substance:
Remark: histopath:
liver: focal necrosis;
pancreas, endocrine: islet enlargement with cell vacuolization, peri-islet congestion;
pancreas, exocrine: occasional pyknotic nuclei, acinar atrophy, and periacinar inflamatory cell infiltrate.
Result: 1) 151/171 mg/kg/day M/F:
NOEL
no effects
2) 381/422 mg/kg/day M/F:
kidney weight, incr;
urinary pH, decr;
kidney weight, incr.
3) 960/1069 mg/kg/day M/F:
kidney weight, incr;
urinary pH, decr;
kidney weight, incr;
liver weight, incr (F);
blood, RBC, decr;
liver, histopath;
pancreas, histopath.
Source: Monsanto Europe N.V. Bruxelles

(124)

Species: rat **Sex:** male
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 182 days
Frequency of treatment: daily
Post. obs. period: no
Doses: 0.03, 0.09, 0.28, 0.83, 2.5 %
Control Group: yes
NOAEL: = 470 mg/kg bw
Method: Directive 84/449/EEC, B.7 "Sub-acute toxicity (oral)"
Year: 1984 **GLP:** no data
Test substance: other TS
Remark: .03, .09, .28, .83, 2.5% = 17, 51, 159, 470, and 1417 mg/kg/day
histopath:
testes: hypospermia.
testes: atrophy of seminiferous tubules.
epididymis: hypospermia.
prostate: focal atrophy.
Result: 1) 17 mg/kg/day:
no effects
2) 51 mg/kg/day:
no effects
3) 159 mg/kg/day:
no effects
4) 470 mg/kg/day:
no effects
NOEL
5) 1417 mg/kg/day:
body weight, decr;
testes, weight, decr;
testes, histopath;
epididymis, histopath;
prostate, histopath;
kidney, histopath;
blodd, red cell mass, decr;
blood, hemoglobin, decr;
blood, RBC, decr;
blood, hematocrit, decr;
Source: Monsanto Europe N.V. Bruxelles
Test substance: purity > 96%

(125)

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: daily
Frequency of treatment: 21 days
Post. obs. period: no
Doses: 0.6, 1.2, 2,5 %
Control Group: yes
LOAEL: = 639 mg/kg bw
Method: other
Year: 1985 **GLP:** yes
Test substance:
Remark: 5 rats/sex/group;
dose based on actual food intake;
liver enzymes
PCoA oxidase, layric acid 11-hydroxylase and lauric acid 12-hydroxylase;
histopath
liver: peroxisome proliferation
testes: atrophy.
Result: 1) 0.6%
LOEL
liver enzyme, incr,M.
2) 1.2%
body weight, decr,M;
liver enzyme, incr,.
3) 2.5%
body weight, decr,M;
food consumption, decr;
liver weight, incr;
kidney weight; incr;
testes weight, decr;
liver, histopath;
testes, histopath.
Source: Monsanto Europe N.V. Bruxelles

(126)

Species: rat **Sex:** female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 365 days
Frequency of treatment: daily
Post. obs. period: no
Doses: 0.6 and 1.2%
Control Group: yes
LOAEL: = 360 mg/kg bw
Method: other
Year: 1994 **GLP:** yes
Test substance:
Remark: 0.6% and 1,2% in diet = 360 and 720 mg/kg/day using a conversion factor of 600;
Female rats were fed diets containing 0.6 and 1.2% BBP for one year. Cell proloferation was measured at 1 week, 3 months and 12 months. Peroxisome proliferation was measured at 1 and 12 months. Immune status was assessed at 1 and 12 months.
liver enzyme:
carnitine acetyltransferase, palmityl CoA oxidase.
Result: 1) 0.6%
liver enzyme, incr.
2) 1.2%
liver enzyme, incr.
Source: Monsanto Europe N.V. Bruxelles

(127)

Species: rat **Sex:** male
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 28 days
Frequency of treatment: daily
Post. obs. period: none
Doses: .01, ,05, .1, .5, 1 %
Control Group: yes
NOAEL: = 540 mg/kg bw
Method: other
Year: 1992 **GLP:** yes
Test substance: other TS
Remark: liver enzyme:
CN insensitive palmitoyl CoA oxidase;
no histopathological findings in the liver abd testes
Result: 1) .01%
no effects
2) .05%
no effects
3) .1%
no effects
4) .5%
NOEL for peroxisome proliferation
body weight, decr.
5) 1%

body weight, decr;
liver weight, incr;
liver enzyme, incr.

Source: Monsanto Europe N.V. Bruxelles

Test substance: purity=98.1%

(128)

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: 160, 480, 1600 mg/kg bw/day
Control Group: yes
NOAEL: = 160 mg/kg bw
Method: other
Year: **GLP:** no
Test substance:
Remark: histopath:
testes, atrophy.(note: only minimal changes (<5% of tubules affected) were observed in 1/6 rats from the mid-dose group)
Result: 1) 160 mg/kg/day:
NOEL
no effects
2) 480 mg/kg/day:
testes, atrophy.
3) 1600 mg/kg/day:
testes, histopath.
Source: Monsanto Europe N.V. Bruxelles

(121)

Species: rat **Sex:** male
Strain: Wistar
Route of admin.: gavage
Exposure period: 14 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 480,1600 mg/kg bw/day
Control Group: yes
NOAEL: = 480 mg/kg bw
Method: other
Year: **GLP:** no
Test substance:
Result: 1) 480 mg/kg/day:
no effects
NOEL
2) 1600 mg/kg/day
body weight, decr;
testes, atrophy.
Source: Monsanto Europe N.V. Bruxelles

(121)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 14 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 1600, 3100, 6300, 12500, 2500 ppm
Control Group: yes
NOAEL: > 5250 mg/kg bw
Method: other
Year: 1982 **GLP:** no
Test substance:
Remark: 1600, 3100, 6300, 12500, 25000 ppm = 336, 651, 1323, 2625, and 5250 mg/kg/day using a conversion factor of 0.21; 5 animals/sex/group
Result: 1) 1600 ppm
no effects
2) 3100 ppm
no effects
3) 6300 ppm
no effects
4)12500 ppm
no effects
5) 25000 ppm
NOEL
no effects
Source: Monsanto Europe N.V. Bruxelles

(109)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 90 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 1600, 3100, 6300, 12500 ppm
Control Group: yes
NOAEL: = 882 mg/kg bw
LOAEL: = 224 mg/kg bw
Method: other
Year: 1982 **GLP:** no
Test substance:
Remark: 1600, 3100, 6300, 12500, 25000 ppm = 224, 434, 882, 1750, 3500 mg/kg/day using a conversion factor of .14
Result: 1) 1600 ppm
LOEL
body weight, decr,M
2) 3100 ppm
body weight, decr,M
3) 6300 ppm
body weight, decr,M.
4) 12500 ppm
body weight, decr.

5) 25000 ppm
body weight, decr.

Source: Monsanto Europe N.V. Bruxelles

(109)

Species: dog **Sex:** male/female
Strain: Beagle
Route of admin.: oral unspecified
Exposure period: 90 days
Frequency of treatment: daily
Post. obs. period: none
Doses: 1.0, 2.0, and 5.0 %
Control Group: yes
NOAEL: = 500 mg/kg bw
Method: other
Year: **GLP:** no
Test substance:
Remark: 1, 2, 5% = 250, 500, 1250 mg/kg/day using a conversion factor of 250.
Dogs were fed diets containing 1,2, and 5% BBP for 90 days. As a result of palatability problems the high dose was given in capsules. Hematology (hemoglobin, packed cell volume, erythrocyte count, total and differential leukocyte count) and urinalysis were performed at monthly intervals. Liver and kidney function was also measured at these times. All dogs were subjected to a gross necropsy and histopathological evaluation was performed on 30 tissues,

Result: 1) 1%
no effects
2) 2%
no effects
NOEL
3) 5%
body weight, decr.

Source: Monsanto Europe N.V. Bruxelles

(129)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium
Concentration: 0.1, 1.0, 5.0, 10 microliters/plate
Metabolic activation: with and without
Result: negative
Method: other
Year: 1976 **GLP:** no
Test substance:
Remark: no cytotoxicity
number of replicates: 1

Source: Monsanto Europe N.V. Bruxelles

(130)

Type: Ames test
System of testing: Salmonella typhimurium TA99,TA100, TA1535, TA1537, TA1538
Concentration: up to 10 ul/plate
Metabolic activation: with and without
Result: negative
Method: other
Year: 1976 **GLP:** no
Test substance:
Remark: no cytotoxicity
number of replicates: 1
Source: Monsanto Europe N.V. Bruxelles
(131)

Type: Cytogenetic assay
System of testing: CHO cells
Concentration:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1987 **GLP:** no data
Test substance:
Source: Monsanto Europe N.V. Bruxelles
(132)

Type: DNA damage and repair assay
System of testing: Bacilus subtilis (rec A-)
Concentration: 30 mg/plate
Metabolic activation:
Result: negative
Method: other
Year: 1976 **GLP:** no data
Test substance:
Source: Monsanto Europe N.V. Bruxelles
(133)

Type: DNA damage and repair assay
System of testing: Escherichia coli (uvrA-, polA-,recA-)
Concentration: 30 mg/plate
Metabolic activation: no data
Result: negative
Method: other
Year: 1975 **GLP:** no data
Test substance:
Source: Monsanto Europe N.V. Bruxelles
(133)

Type: Escherichia coli reverse mutation assay
System of testing: Escherichia coli (wild, uvrA-)
Concentration: 30 mg/plate
Metabolic activation: no data
Result: negative
Method: other
Year: 1975 **GLP:** no data
Test substance:
Source: Monsanto Europe N.V. Bruxelles

(133)

Type: Mouse lymphoma assay
System of testing: L5178Y mouse lymphoma cells
Concentration: up to 1.25 ul/ml
Metabolic activation: with and without
Result: negative
Method: other
Year: 1976 **GLP:** no
Test substance:
Remark: cytotoxicity was observed at 1.25 ul/ml
number of replicates: 1
Source: Monsanto Europe N.V. Bruxelles

(134)

Type: Sister chromatid exchange assay
System of testing: CHO cells
Concentration: up to 1250 ug/ml
Metabolic activation: with and without
Result: ambiguous
Method: other
Year: 1987 **GLP:** no data
Test substance:
Remark: ambiguous results -S9
negative results +S9
slight evidence for a trend in one of two SCE tests
Source: Monsanto Europe N.V. Bruxelles

(132)

Type: other
System of testing: Balb/3T3 cells
Concentration: up to 0.16 ul/ml
Metabolic activation: without
Result: negative
Method: other
Year: 1985 **GLP:** yes
Test substance:
Remark: In vitro transformation of Balb/373 cells
cytotoxicity seen at all concentrations
number of replicates: 1

Source: Monsanto Europe N.V. Bruxelles

(135)

5.6 Genetic Toxicity 'in Vivo'

Type: Dominant lethal assay
Species: mouse **Sex:** male
Strain: other: B6C3F1 and CD-1
Route of admin.: s.c.
Exposure period: three times during 10 days
Doses: 400-600, 1280-1840, and 3200-4560 mg/kg/day
Result:
Method: other
Year: 1987 **GLP:** no data
Test substance:
Remark: no additional information from abstract
Result: no induction of dominant lethality
Source: Monsanto Europe N.V. Bruxelles

(136)

Type: Drosophila SLRL test
Species: Drosophila melanogaster **Sex:** male
Strain:
Route of admin.: oral feed
Exposure period: 48 hours
Doses: 10000 and 50000 ppm
Result:
Method:
Year: 1985 **GLP:** no data
Test substance:
Remark: if no significant mutagenicity was observed, then BBP was tested by injection (500 ppm). Negative results were obtained.
Result: no indication of resiprocal translocation
Source: Monsanto Europe N.V. Bruxelles

(137)

5.7 Carcinogenicity

Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 24 months
Frequency of treatment: 7 days/week
Post. obs. period: none
Doses: 6000, 12000 ppm
Result:
Control Group: yes
Method: other: National Toxicology Program Method
Year: 1982 **GLP:** no data
Test substance: other TS
Remark: 6000, 12000 ppm = 360, 720 mg/kg bw, the conversion factor is 0.06.
50 rats/dose group
male portion of study terminated at week 30 due to unexplained hemorrhaging. Therefore, BBP not adequately tested for carcinogenicity in males.
histopath:
spleen: splenomegaly
Result: 1) 6000 ppm:
no effects;
NOEL
2) 12000 ppm:
spleen, histopath;
liver, weight, incr;
blood, mononuclear cell leukemia (F).
Source: Monsanto Europe N.V. Bruxelles
Test substance: purity 97.2%

(109)

Species: mouse **Sex:** male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 24 months
Frequency of treatment: 7 days/ week
Post. obs. period: none
Doses: 6000, 12000 ppm
Result:
Control Group: yes
Method: other: National Toxicology Program Method
Year: 1982 **GLP:** no data
Test substance: other TS
Remark: 6000, 12000 ppm = 840, 1680 mg/kg bw, the conversion factor is 0.14.
50 mice/dose group
Result: 1) 6000 ppm:
no effects
2) 12000 ppm:
no effects
NOEL

Source: Monsanto Europe N.V. Bruxelles

(109)

5.8 Toxicity to Reproduction

Type: Fertility
Species: rat **Sex:** male
Strain: Fischer 344
Route of admin.: oral feed
Exposure Period: 26 weeks
Frequency of treatment: daily
Premating Exposure Period male: 26 weeks
Duration of test: 26 weeks
Doses: 0.03, 0.28, 2.5%
Control Group: yes
NOAEL Parental: = 168 mg/kg bw
NOAEL F1 Offspr.: = 168 mg/kg bw
Method: other
Year: 1985 **GLP:** no data
Test substance: other TS
Remark: 0.03, 0.28, 2.5% w/w in diet = 18, 168, 1500 mg/kg/bw/day
doses calculated using a conversion factor of 600
histopath:
testes, aspermia (only at dosage levels exceeding the limit of 1000 mg/kg/day)
reproductive capacity decreased only at dose that produced significant parental toxicity
Result: 1) 18 mg/kg bw/ day:
no effects
2) 168 mg/kg bw/day:
no effects
NOEL
3) 1500 mg/kg bw/day:
body weight, decr;
testis, weight, decr;
testis, histopath;
reproductive capacity, decr.
Source: Monsanto Europe N.V. Bruxelles
Test substance: purity > 98%

(125)

Type: One generation study
Species: rat **Sex:** male/female
Strain: Wistar
Route of admin.: oral feed
Exposure Period: until weaning
Frequency of treatment: daily
Premating Exposure Period
male: 10 weeks
female: 2 weeks
Duration of test: 192 days
Doses: 0.2, 0.4, 0.8
Control Group: yes
NOAEL Parental: = 206 mg/kg bw
NOAEL F1 Offspr.: = 418 mg/kg bw
Method: Directive 87/302/EEC, part B, p. 43 "One-generation reproduction toxicity test"
Year: 1987 **GLP:** yes
Test substance: other TS
Remark: 0.2, 0.4, 0.8% in diet = 108, 206, 418 mg/kg bw/day for M
= 106, 217, 448 mg/kg bw/day for F
Result: 1) 0.2% in diet:
no effects in parents and offspring
2) 0.4% in diet:
no effects in parents and offspring
3) 0.8% in diet:
F0 body weight,decr,F;
F0 liver weight, incr, F;
F1b pup body weight, decr, only on day 21;
no histopathological findings.
Source: Monsanto Europe N.V. Bruxelles
Test substance: purity = 98.1%
a 1:1 blend of two products

(138)

Type: other
Species: rat **Sex:** male
Strain: Fischer 344
Route of admin.: oral feed
Exposure Period: 26 weehs
Frequency of treatment: daily
Premating Exposure Period
male: 26 weeks
Duration of test: 26 weeks
Doses: 0.03, 0.09, 0.28, 0.83, 2.5%
Control Group: yes
NOAEL Parental: = 498 mg/kg bw
Method: other
Year: 1985 **GLP:** no data
Test substance: other TS
Remark: 0.03, 0.28, 2.5% w/w in diet = 18, 54, 168, 498, 1500 mg/kg/bw/day
doses calculated using a conversion factor of 600
histopath:
testes, aspermia (only at dosages exceeding the limit dose of 1000 mg/kg/day)

Result: 1) 18 mg/kg bw/ day:
no effects
2) 54 mg/kg bw/day:
no effects
3) 168 mg/kg bw/day:
no effects
4) 498 mg/kg bw/day:
no effects
NOEL
5) 1500 mg/kg bw/day
body weight, decr;
testis weight, decr;
testis, histopath

Source: Monsanto Europe N.V. Bruxelles

(125)

Type: other
Species: rat **Sex:** male
Strain: Fischer 344
Route of admin.: oral feed
Exposure Period: 14 days
Frequency of treatment: daily
Duration of test: 14 days
Doses: 0.625, 1.25, 2.5, 5.0%
Control Group: yes
NOAEL Parental: = 750 mg/kg bw
Method: other
Year: 1985 **GLP:** no data
Test substance: other TS
Remark: 0.625, 1.25, 2.5, 5.0% = 375, 750, 1500, 3000 mg/kg bw/day
doses based on a conversion factor of 600
histopath:
testis: cell sloughing (only at dosages exceeding the limit dose of 1000 mg/kg/day);
epidiymis: epithelial cell necrosis

Result: 1) 0.625% in diet:
no effects
2) 1.25% in diet:
no effects
3) 2.5% in diet:
body weight, decr;
testis weight, decr;
epididymis weight, decr;
prostate weight, decr;
seminal vesicle weight, decr;
plasma testosterone, decr;
plasma FSH, incr;
bone marrow cellularity, decr;
plasma LH, incr;
testis, histopath;
epididymis, histopath.
5) 5.0% in diet:
body weight, decr;
testis weight, decr;
epidymis weight, decr;
prostate weight, decr;

seminal vesicle weight, decr;
bone marrow cellularity, decr;
plasma testosterone, decr;
plasma FSH, incr;
plasma LH, incr;
testes, histopath;
epididymis, histopath.

Source: Monsanto Europe N.V. Bruxelles

(139)

Type: other
Species: rat **Sex:** male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure Period: 21 days
Frequency of treatment: daily
Premating Exposure Period
male: 14 days
female: 14 days
Duration of test: 14 days
Doses: 0.6, 1.2, 2.5 %
Control Group: yes
NOAEL Parental: <= 679 mg/kg bw
Method: other
Year: 1985 **GLP:** no data
Test substance: other TS
Remark: 0.6, 1.2, 2.5% in diet = 639, 1277, 2450 mg/kg bw/day for males and 679, 1346, 2628 mg/kg bw/day for females
histopath:
testes, atrophy (only at dosages exceeding the limit dose of 1000 mg/kg/day).
Result: 1) 0.6% in diet:
liver weight, incr
2) 1.2% in diet:
body weight, decr (M);
liver weight, incr.
3) 2.5% in diet:
body weight, decr;
liver weight, incr;
testes weight, decr;
testes, histopath.

Source: Monsanto Europe N.V. Bruxelles

(140)

5.9 Developmental Toxicity/Teratogenicity

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: gavage
Exposure period: days 7-15 of gestation
Frequency of treatment: daily
Duration of test: 20 days
Doses: 500, 750, 1000 mg/kg/day
Control Group: yes
NOAEL Maternalt.: = 500 mg/kg bw
NOAEL Teratogen.: = 500 mg/kg bw
Method: other
Year: 1992 **GLP:** no data
Test substance: other TS
Remark: Developmental toxicity seen only at levels producing maternal toxicity,
malformations:
cleft palate
skeletal changes
dilated renal pelvis
Result: 1) 500 mg/kg/day
no effects
NOEL
2) 750 mg/kg/day
maternal body weight, decr;
postimplantation loss, incr;
fetal body weight, decr;
malformations
3) 1000 mg/kg/day
maternal mortality;
maternal body weight, decr;
complete resorption of embryos
Source: Monsanto Europe N.V. Bruxelles
Test substance: purity = 98.2%

(141)

Species: rat **Sex:** female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: days 6-15 of gestation
Frequency of treatment: daily
Duration of test: 20 days
Doses: 0.5, 1.25, 2.0%
Control Group: yes
NOAEL Maternalt.: = 420 mg/kg bw
NOAEL Teratogen.: = 1100 mg/kg bw
Method: Directive 87/302/EEC, part B, p. 24 "Teratogenicity test - rodent and non-rodent"
Year: 1987 **GLP:** no data
Test substance: other TS
Remark: Developmental toxicity seen onl at levels producing maternal toxicity and the Limit Dose (1000 mg/kg),
0.5, 1.25, 2.0% = 420, 1100, 1640 mg/kg bw
external malformation: eye;
visceral malformaton: urogenital system; great vessels of heart;
skeletal malformation; axial skeleton.
Result: 1) 0.5% in diet:
maternal NOEL
developmental NOEL
2) 1.25% in diet:
maternal:
body weight,decr;
offspring:
body weight decr.
3) 2.0% in diet:
maternal:
body weight, decr;
offspring:
fetus,weight,decr;
resorptions, incr;
fetus, external malformations;
fetus, visceral malformations;
fetus, skeletal malformations.
Source: Monsanto Europe N.V. Bruxelles
Test substance: purity = 96%

(142)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: oral feed
Exposure period: days 0-20 of gestation
Frequency of treatment: daily
Duration of test: 20 days
Doses: 0.25, 0.5., 1.0, 2.0%
Control Group: yes
NOAEL Maternalt.: = 314 mg/kg bw
NOAEL Teratogen.: > 1018 mg/kg bw
Method: other
Year: 1990 **GLP:** no data
Test substance: other TS
Remark: Developmental toxicity seen only at levels producing marked maternal toxicity and the Limit Dose (1000 mg/kg),
The author's dose (ie., 185, 375, 654, 974) were based on initial body weight. We recalculated these doses (ie., 152, 314, 568, 1018) based on average body weight during the treatment period.
Result: 1) 0.25% in diet:
no effects
2) 0.5% in diet:
offspring:
no malformations.
3) 1.0% in diet:
maternal:
body weight, decr;
offspring:
body weight, decr;
no malformations
4) 2.0% in diet:
maternal:
body weight, decr;
offspring:
complete resorptions.
Source: Monsanto Europe N.V. Bruxelles

(143)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: oral feed
Exposure period: days 0-20 of gestation
Frequency of treatment: daily
Duration of test: 20 days
Doses: 2%
Control Group: yes
NOAEL Maternalt.: < 1087 mg/kg bw
NOAEL Teratogen.: > 1087 mg/kg bw
Method: other
Year: 1991 **GLP:** no data
Test substance: other TS
Remark: Developmental toxicity seen only at doses that produced maternal toxicity and the Limit Dose (1000 mg/kg)
2.0% in diet = 1087 mg/kg/d (based on average body weight during the treatment period). The author reported a dose of 974 mg/kg/d, which was based on body weight at the start of yreatment.
Result: 2%
maternal weight, decr;
maternal food consumption, decr;
embryo lethality
Source: Monsanto Europe N.V. Bruxelles

(144)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: oral feed
Exposure period: various: 0-20, 0-7, 7-16, 16-20 days of gestation
Frequency of treatment: daily
Duration of test: 20 days
Doses: 2%
Control Group: yes
NOAEL Maternalt.: < 824 mg/kg bw
NOAEL Teratogen.: < 824 mg/kg bw
Method: other
Year: 1992 **GLP:** no data
Test substance: other TS
Remark: Developmental toxicity seen only at levels producing maternal toxicity,
2% in diet is equivalent to about 1022 (days 0-20), 589 (days 0-7), 824 (days 7-16), and 557 (days 16-20) mg/kg/day based on average body weight during the treatment period.
malformations:
cleft palate
fusion of the sternebrae
Result: 1) days 0-20
maternal body weight, decr;
complete resorption of ebryos
2) days 0-7
maternal body weight, decr;
postimplantation loss, incr;
3) days 7-16
maternal body weight, decr;

postimplantation loss, incr;
fetal malformations
4) days 16-20
maternal body weight, decr;
fetal body weight, decr.

Source: Monsanto Europe N.V. Bruxelles
Test substance: 98.2 % purity

(145)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: oral feed
Exposure period: various: days 0-20, 0-11, 11-20 of gestation
Frequency of treatment: daily
Duration of test: 20 days
Doses: 2%
Control Group: yes
NOAEL Maternalt.: < 631 mg/kg bw
NOAEL Teratogen.: < 631 mg/kg bw
Method: other
Year: 1992 **GLP:** no
Test substance: other TS
Remark: Developmental toxicity seen only at levels that produced maternal toxicity,
2% in diet = 1022 (days 0-20), 791 (days 0-11), and 631 (days 11-20) mg/kg/day, based on average body weight during the treatment period.
malformations:
cleft palate
fusion of the sternebrae
Result: 1) days 0-20
maternal weight, decr;
complete resorption of embryos
2) days 0-11
maternal weight, decr;
complete resorption of embryos.
3) days 11-20
maternal weight, decr;
fetal body weight, decr;
malformations
Source: Monsanto Europe N.V. Bruxelles
Test substance: purity = 98.2%

(146)

Species: rat **Sex:** female
Strain: Wistar
Route of admin.: oral feed
Exposure period: days 7-9, 10-12, or 13-15 of gestation
Frequency of treatment: daily
Duration of test: 20 days
Doses: 600,750,1000 mg/kg/d
Control Group: yes
NOAEL Teratogen.: = 600 mg/kg bw
Method: other
Year: 1993 **GLP:** no data
Test substance: other TS
Remark: Developmemtal effects seen only at levels previously shown to produce maternal toxicity (no data available in this reference),
malformations:
skeletal
cleft palate
Result: 1) 600 mg/kg/day on days 13-15
no effects
2) 750 mg/kg/day on days 10-12
postimplantation loss, incr;
fetal body weight, decr;
malformations
3) 1000mg/kg/day on days 7-9
postimplantation loss, incr;
fetal body weight, decr;
malformations
Source: Monsanto Europe N.V. Bruxelles
Test substance: purity = 98.2%

(147)

Species: mouse **Sex:** female
Strain: CD-1
Route of admin.: oral feed
Exposure period: days 6-15 of gestation
Frequency of treatment: daily
Duration of test: 19 days
Doses: 0.1, 0.5, 1.25, 2.0%
Control Group: yes
NOAEL Maternalt.: = 182 mg/kg bw
NOAEL Teratogen.: = 182 mg/kg bw
Method: Directive 87/302/EEC, part B, p. 24 "Teratogenicity test - rodent and non-rodent"
Year: 1987 **GLP:** no data
Test substance: other TS
Remark: Developmental toxicity seen only at levels producing maternal toxicity,
0.1, 0.5, 1.25, 2.0% = 182, 910, 2330, 4120 mg/kgbw/day
Result: 1) 0.1% in diet:
no effects
2) 0.5% in diet:
maternal:
body weight, decr;
liver weight, incr;

kidney weight, incr;
offspring:
resorptions, incr;
live litter size, decr;
body weight, decr;
malformations, incr.
3) 1.25% in diet:
maternal:
body weight, decr;
liver weight, incr;
kidney weight, incr;
offspring:
resorptions, incr;
live litter size, decr;
body weight, decr;
malformations, incr.
4) 2.0% in diet:
maternal:
body weight, decr;
all litters resorbed

Source: Monsanto Europe N.V. Bruxelles
Test substance: purity = 96%

(142)

Species: rabbit **Sex:** female
Strain: New Zealand white
Route of admin.: oral unspecified
Exposure period: days 6-18 of gestation
Frequency of treatment: daily
Duration of test:
Doses: 3,10 mg/kg bw
Control Group: yes
NOAEL Maternalt.: = 10 mg/kg bw
NOAEL Teratogen.: = 10 mg/kg bw
Method: other
Year: 1976 **GLP:** no
Test substance:
Remark: Higher doses of 30-300 mg/kg bw/day caused maternal weight loss and early fetal deaths
Result: 1) 3 mg/kg:
no effects
2) 10 mg/kg
no effects
Source: Monsanto Europe N.V. Bruxelles

(148)

5.10 Other Relevant Information

Type: adsorption
Remark: About 30 % of the dose was excreted in the urine and feces within 7 days. About 45 % of the dose remained at the application site.
male Fischer 344 rats received a single dermal application of 30-40 mg/kg (5-8 mg/cm2) of 14C-BBP on their backs. The BBP was applied in ethanol. The site was clipped of hair

prior to application and covered with a perforated cap after treatment. The rats were restrained and housed for 7 days in metabolic cages to collect urine and feces.

Source: Monsanto Europe N.V. Bruxelles

(149)

Type: Chemobiokinetics general studies

Remark: male Fischer 344 rats were dosed with 14C-BBP at 2, 20, 200, or 2000 mg/kg orally or 20 mg/kg intravenously.
urine, feces, bile, and tissues were collecred at intervals and analyzed for parent compound and metabolites.

Source: Monsanto Europe N.V. Bruxelles

(150)

Type: Chemobiokinetics general studies

Remark: Excreted about 80 % of the radioactivity in the urine and about 20 % in the feces.

Source: Monsanto Europe N.V. Bruxelles

(151)

Type: Neurotoxicity

Remark: 1) 500 mg/kg bw/day: no effects; NOEL
2) 1500 mg/kg bw/day: body weight, decr.
3) 3000 mg/kg bw/day: body weight, decr; hindlimb, stiffness, incr.
CD rats (10/sex/group) received 500, 1500, and 3000 mg/kg bw/d for 6 weeks. Afterwards, rats were evaluated for neuropathological changes.

Source: Monsanto Europe N.V. Bruxelles

(152)

5.11 Experience with Human Exposure

Remark: workers in a PVC processing plant, exposed to diisodecyl phthalate and/or butylbenzyl phthalate in the air, showed statistically higher levels of phthalate acid ester (not specified) in urine than workers of the control group; contrary to earlier finding no clinically obvious cases of polyneuropathy were detected.

Source: Monsanto Europe N.V. Bruxelles

(153)

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(2) Ref 1:" Plasticizers -A consideration of their impact on Health and the Environment"-publ.CEFIC-Brussels (1989)

Ref 2:Cadogan,D.F.,Papez,M.,Poppe,A.C.,Pugh,D.M.and Scheubel J.B.-"An Asessment of the Release,Occurence,and Possible Effects of Phthalate Plasticizers in the Environment"- Paper at PVC 93 Conference-Inst.of Materials(April 1993)

Ref 3:Gledhill ,W.E.,--internal report-Environmental Safety Assessment-Benzyl phthalates-April 1991.

Ref 4:Furtmann ,W.R.-"Phthlate in Der Aquatischen Umwelt" Landesamt fur Wasser und Abfall Nordrhein-Westfalen(1993).

Ref 5:Hurford,N et al,"Concentrations of Chemicals in the North Sea due to Operational Discharges form Chemical Tankers-Results form Second Survey,October 1988-" Oil and Chem' Pollution 7(1990) 251-270

(3) Gledhill WE et al;Env Sci Tech 14:301-5 1980.

(4) (1) -Monsanto internal data

(5) (2)Bayer AG-internal data

(6) (2)-Bayer AG internal data

(7) (1)-Monsanto internal data

(8) Monsanto internal data

(9) (3)Bayer AG-internal data -Leverkusen 1987

(10) Bayer AG-internal data-Leverkusen 1987

(11) Howard,P.H.,Banerjee,S,and Robillard,K.H., "Measurement of Water Solubilities,Octanol/Water Partition Coefficients and Vapour Pressures of Commercial Phthalate Esters" Environmental Toxicity and Chemistry Vol.4,page 653-661

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(18) Bayer AG-internal data

(19) Monsanto report ES-80-SS04

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Verschureren, K. (1983), Handbook of Environmental Data on Organic Chemicals. Van Nostrand Reinhold Company, Inc. NY

(20) Monsanto report MO-85-9169

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(21) Gledhill, W.E. et al. (1980), An environmental safety assessment for butyl benzyl phthalate, Environmental Science and Technology 14(3), 301-305.

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7.1 Risk Assessment

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IUCLID

Data Set

Existing Chemical	:	ID: 68515-48-0
CAS No.	:	68515-48-0
EINECS Name	:	1,2-Benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich
EINECS No.	:	271-090-9
Molecular Weight	:	418
Structural Formula	:	c(ccc1C(=O)OCC(C)CCC(C)CC)cc1C(=O)OCC(C)CCC(C)CC
Molecular Formula	:	C26O4H42

Producer Related Part

Company	:	Exxon Chemical Holland BV
Creation date	:	21.12.1992

Substance Related Part

Company	:	Exxon Chemical Holland BV
Creation date	:	21.12.1992
Memo	:	
Printing date	:	13.11.2001
Revision date	:	21.12.1992
Date of last Update	:	15.10.2001
Number of Pages	:	67
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

Substance type : organic
Physical status : liquid
Purity : > 99.7 - % w/w
Remark : C8-C10 branched alkyl ester, C9 rich, with an average of 9.2 carbons per alkyl chain.
Smiles code for typical isomer.

12.02.1996

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

Diisononyl Phthalate
Remark : In the "oxo" Industry, the term "iso" is used for designating a complex substance containing isomeric constituents and does not refer to the IUPAC definition.

26.04.2001

DINP
22.12.1992

Jayflex DINP
22.12.1992

1.3 IMPURITIES

CAS-No :
EINECS-No :
EINECS-Name : Diisononyl ether
Contents : - % w/w
29.01.1996

CAS-No :
EINECS-No :
EINECS-Name : Isononyl benzoate
Contents : - % w/w
Remark : Diisononyl ether and Isononyl benzoate content ca. 0.07% w/w
The above mentioned impurities have been identified.

30.01.1996

CAS-No	:	68526-84-1
EINECS-No	:	
EINECS-Name	:	Isononyl alcohol
Contents	:	ca. .05 - % w/w

30.01.1996

1.4 ADDITIVES

CAS-No	:	80-05-7
EINECS-No	:	
EINECS-Name	:	Phenol, 4.4'-(1-methylethylidene)bis
Contents	:	= .15 - % w/w
Remark	:	On specific request from customers 0.15% w/w bis phenol A is added to DINP.

02.02.1996

1.5 QUANTITY

Production during the last 12 months	:	
Import during the last 12 months	:	
Quantity produced	:	tonnes in
Remark	:	Please refer to proprietary document for description of quantities produced.

20.03.1996

1.6.1 LABELLING

Labelling	:	no labelling required (no dangerous properties)
Nota	:	
Specific limits	:	no data
R-Phrases	:	
S-Phrases	:	
Remark	:	This product does not require an environmental label.

24.11.1997

1.6.2 CLASSIFICATION

Classification	:	no classification required (no dangerous properties)
Class of danger	:	
R-Phrases	:	
Remark	:	This product does not require an environmental classification.

24.11.1997

1.7 USE PATTERN

Type	:	type
Category	:	Use resulting in inclusion into or onto matrix

02.02.1996

Type : industrial
Category : Polymers industry
29.01.1996

Type : industrial
Category : other: plasticizer
02.02.1996

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit : MAC (NL)
Limit value : 5 mg/m3
12.02.1996

Type of limit : OES (UK)
Limit value : 5 mg/m3
29.01.1996

Type of limit : TLV (US)
Limit value : 5 mg/m3
Short term exposure
Limit value : 10 mg/m3
Schedule : 15 minute(s)
Frequency : 1 times
Remark : Data for Di-2-Ethylhexyl phthalate
12.02.1996

Type of limit : other
Limit value : 5 mg/m3
Remark : Exxon recommended Occupational Exposure Limit
12.02.1996 (77)

Type of limit : other: MAK (Germany)
Limit value : 10 mg/m3
Remark : Data for Di-2-ethylhexyl phthalate
12.02.1996

Type of limit : other: OEL (Finland)
Limit value : 5 mg/m3
Remark : Data for Di-2-Ethylhexyl phthalate
29.01.1996

Type of limit : other: OEL (Norway)
Limit value : 3 mg/m3
Remark : Data for Di-2-Ethylhexyl phthalate
29.01.1996

Type of limit : other: OEL (Sweden)
Limit value : 3 mg/m3
29.01.1996

Type of limit : other: TLV (DE)
Limit value : 3 mg/m3
Remark : Data for Di-2-ethylhexyl phthalate
12.02.1996

Type of limit : other: VME (France)
Limit value : 5 mg/m3
Remark : Data for Di-2-Ethylhexyl phthalate
29.01.1996

1.9 SOURCE OF EXPOSURE

Remark : The manufacturing process for DINP is within a closed system under vaccuum. The different sources of exposure during manufacturing, distribution, processing use and disposal are described in detail by Cadogan, et al. (1994). Further information on the use of plasticizers and general equipment and process description can be found in the additional references cited below:
29.07.1998 (33) (78) (96) (109) (121) (130) (146) (151)

1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES

1.10.2 EMERGENCY MEASURES

1.11 PACKAGING

1.12 POSSIB. OF RENDERING SUBST. HARMLESS

1.13 STATEMENTS CONCERNING WASTE

1.14.1 WATER POLLUTION

1.14.2 MAJOR ACCIDENT HAZARDS

1.14.3 AIR POLLUTION

1.15 ADDITIONAL REMARKS

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value	:	= -48 - ° C
Sublimation	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	pour point
Source	:	Exxon Biomedical Sciences, Inc.

01.06.2001 (73)

2.2 BOILING POINT

Value	:	> 250 - ° C at
Decomposition	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Exxon Biomedical Sciences, Inc.

01.06.2001 (73)

2.3 DENSITY

Type	:	density
Value	:	= .972 - g/cm3 at 20° C
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Exxon Biomedical Sciences, Inc.

01.06.2001 (73)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	< .01 - hPa at 20° C
Decomposition	:	
Method		
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Exxon Biomedical Sciences, Inc.

01.06.2001 (73)

Value	:	= .0000000681 - hPa at 25° C
Decomposition	:	
Method		
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Source : ExxonMobil Biomedical Sciences, Inc.
05.06.2001 (40)

Value : = .00000072 - hPa at 25° C
Decomposition :
Method other (measured): US EPA Federal Register 45:77345-77350
Year : 1980
GLP : no data
Test substance :
Remark : Mean value measured at 3 different flow-rates.
Source : Exxon Biomedical Sciences, Inc.
29.07.1998 (85)

2.5 PARTITION COEFFICIENT

Log pow : > 8 - at 25° C
Method other (measured): Draft ASTM Standard (HPLC retention time)
Year :
GLP : no data
Test substance :
Remark : Value not reported for DINP. Report states the higher molecular weight phthalate esters have a different correlation between HPLC retention time and Pow than do the standards (halogenated aromatics). The report also states that the Pow for DEHP by this RP-HPLC method is approximately 3 logs higher than other methods (i.e., OECD Partition Method).
Source : Exxon Biomedical Sciences, Inc.
29.07.1998 (85)

Log pow : = 8.6 - at 25° C
Method
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : ExxonMobil Biomedical Sciences, Inc.
05.06.2001 (40)

Log pow : 9.3 - at ° C
Method other (measured): RP-HPLC retention time.
Year :
GLP : no data
Test substance :
Remark : This value was extrapolated above the regression line (retention time vs Kow) developed for the standards (highest standard = log Pow 5.7). Report states method has been proved reliable for a Kow range of 0-6.
Source : Exxon Biomedical Sciences, Inc.
Test substance : "C8/C10 Phthalate Ester"
29.07.1998 (129)

2.6.1 WATER SOLUBILITY

Value : = .61 - other: ug/l at 21 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other: Slow Stir Procedure

Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A slow stir procedure was used. 100mg DINP was added to a closed carboy containing 12L of carbon-treated water that was then slowly stirred. The aqueous phase was sampled on days 1, 3, and 9 by extraction with a C18 extraction disk. Analysis was by gas chromatography with mass selective detection in the selective monitoring mode.
Source	:	Exxon Biomedical Sciences, Inc.

01.06.2001 (68)

Value	:	= .00031 - at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Remark	:	QSPR estimate
Source	:	ExxonMobil Biomedical Sciences, Inc.

05.06.2001 (40)

Value	:	= .2 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other: (measured) US EPA TSCA
Year	:	1979
GLP	:	
Test substance	:	
Remark	:	Due to experimental difficulties associated with this method when applied to poorly water soluble materials the results of this study significantly overestimate the true water solubility by several orders of magnitude.

03.05.2001 (85)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 214 ° C
Type	:	closed cup
Method	:	other: ASTM D93
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Exxon Biomedical Sciences, Inc.

01.06.2001 (73)

2.8 AUTO FLAMMABILITY

Value	:	= 380 - ° C at
Method	:	other: ASTM E659
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	autoignition temperature
Source	:	Exxon Biomedical Sciences, Inc.

01.06.2001 (73)

2.9 FLAMMABILITY

Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	This product can burn only upon heating to temperatures at or above the flash point.
Source	:	Exxon Biomedical Sciences, Inc.

01.06.2001 (73)

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

Result	:	other: not applicable
Remark	:	Phthalate esters have no known oxidizing properties.

30.01.1996

2.12 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spect.	:	- nm
Rel. intensity	:	- based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	= .0000000000234 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Calculated rate constant for DINP. The calculated half-life from this calculated degradation rate is 5.5 hours, based on an average OH- concentration of 1.5E6 molecules/cm3.
Source	:	Exxon Biomedical Sciences, Inc.

28.07.1998 (55)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	- at degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	
Method	:	other
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Phthalate esters are subject to abiotic hydrolysis at slow rates. Hydrolysis rates are reported to decrease and corresponding half-lives increase with increasing alcohol chain length. Data summarized by Staples et al. conclude that abiotic hydrolysis is unlikely to be an important fate process for phthalate esters under typical environmental conditions (Schwartzenbach et al., 1992, Environmental Organic Chemistry, John Wiley & Sons, NY, NY, USA).
Source	:	Exxon Biomedical Sciences, Inc.

03.05.2001 (138)

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

Type of measurement	:	background concentration
Medium	:	sediment
Method	:	
Concentration	:	-
Remark	:	Sediments from 8 lakes in Sweden and 10 sampling locations in a Swedish river system, which provided a gradient of

anthropogenic influence, were analyzed for DINP in 1994. A total of 54 sediment analyses were performed on samples obtained from these locations. DINP was not detected in any samples (Estimated detection limit <0.02 mg/kg dry wt.).

29.07.1998 (117)

Type of measurement : background concentration
Medium : sediment
Method :
Concentration : -
Remark : Sediments from five large rivers (Rhine, Waal, Maas, W. Schelde, Yssel) and five small rivers (Reeuwijk, Vinkeveense plassen, ringvaart, Nieuwkoopse plassen, Brassemermeer) were analyzed for DINP in 1992. Sediment concentrations in large rivers ranged from <0.1-0.2 mg/kg dry wt. (n=10). DINP in sediments from small rivers was not detected (<0.1 mg/kg dry wt., n=10).

29.07.1998 (131)

Type of measurement : background concentration
Medium : sediment
Method :
Concentration : -
Remark : Sediments from drainage channels next to motorways were sampled in 1992-1993. DINP concentrations ranged from <0.1-0.8 mg/kg dry wt. near new/quiet roads (n=7). The concentration in one sample collected near an old/busy road was 6.7 mg/kg dry wt. (n=1).

29.07.1998 (131)

Type of measurement : background concentration
Medium : sediment
Method :
Concentration : -
Remark : Sediments were collected from four sites on the Rhine River and three sites on the Necker River in Germany. Geometric mean DINP concentrations for the Rhine and Necker rivers were 0.28 (0.03-1.46) and 0.71 (0.43-1.46) mg/kg dry wt., respectively.

29.07.1998 (101)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration : -
Remark : Surface water samples collected from four Japanese rivers and two coastal locations were analyzed in 1994. DINP was not detected in any sample (<5 ug/l, n=28).

29.07.1998 (141)

Type of measurement : background concentration
Medium : ground water
Method :
Concentration : -
Remark : Groundwater samples from four Japanese cites were analyzed in 1993-1994. DINP was not detected in any sample (<5 ug/l, n=18).

29.07.1998 (141)

Type of measurement : background concentration
Medium : drinking water
Method :

Concentration : -
Remark : Drinking water samples from four Japanese cities were analyzed in 1993-1994. DINP was not detected in any sample (<5 ug/l, n=12).

30.07.1998 (141)

Type of measurement : concentration at contaminated site
Medium : sediment
Method :
Concentration : -
Remark : Sediments were collected downstream of two point source discharges in 1994. The mean DINP concentration below one point source was 150 (+/- 124) mg/kg dry wt and ranged from 16 to 314 mg/kg dry wt. based on the analysis of three samples. DINP was not detected below the other point source, i.e. <0.02 mg/kg dry wt. in three samples. DINP was not detected in sediment at stations upstream of both point sources.

29.07.1998 (117)

Type of measurement : concentration at contaminated site
Medium : sediment
Method :
Concentration : -
Remark : Sediments near point source were sampled in 1992-1993. DINP concentrations were below detection (<0.1 mg/kg dry wt., n=11).

29.07.1998 (131)

Type of measurement : concentration at contaminated site
Medium : other: Primary sludge from municipal wastewater treatment plants
Method :
Concentration : -
Remark : Duplicate samples from four wastewater treatment plants were analyzed in 1992-1993. DINP concentrations from two plants located in rural areas were <2 and 41 ug/l (or approximately <1 mg/kg dry wt. and 21 mg/kg dry wt., respectively). DINP concentrations at two plants located in urban areas were <2 and 6.2 ug/l (or approximately 2 mg/kg dry wt. and 7.8 mg/kg dry wt., respectively).

29.07.1998 (131)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : adsorption
Media : water - soil
Air (level I) :
Water (level I) :
Soil (level I) :
Biota (level II / III) :
Soil (level II / III) :
Method : other: USEPA 796.2750 Sediment and Soil Adsorption Isotherm
Year : 1989
Remark : Log Koc for DIDP (diisodecyl phthalate) = 5.46. This is the mean Koc measured for 3 soil types. The Koc for the 3 soils tested ranged from 5.04 to 5.78.
The amount of 14C PAE adsorbed to the soil (ug) was calculated by subtracting the mass of chemical in supernatant plus that adsorbed to the glass after equilibration from the intial mass in solution.

Source : Exxon Biomedical Sciences, Inc.
Test substance : DIDP - Diisodecyl Phthalate
31.03.1998 (152)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year :
Remark : The following calculated values apply to DINP:
51.67% - soil
48.22% - sediment
0.08% - suspended solids
0.03% - biota
Source : Exxon Biomedical Sciences, Inc.
03.08.1998 (17)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, non-adapted
Concentration : 24mg/l related to Test substance
related to
Contact time :
Degradation : = 57 - % after 28 day
Result :
Deg. Product :
Method : OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year : 1993
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Exxon Biomedical Sciences, Inc.
28.07.1998 (64)

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 100mg/l related to Test substance
related to
Contact time :
Degradation : = 71 - % after 28 day
Result :
Deg. Product :
Method : OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Source : Exxon Biomedical Sciences, Inc.
30.07.1998 (16)

Type : aerobic
Inoculum : activated sludge, domestic, non-adapted
Concentration : 45.3mg/l related to Test substance
related to
Contact time :

Degradation	:	= 71 - % after 28 day
Result	:	
Kinetic of test substance	:	10 day = 2.3 - % 11 day = 7.8 - % 12 day = 14.8 - % 21 day = 59.1 - % 22 day = 61.2 - %
Deg. Product	:	
Method	:	OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year	:	1993
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	O2 consumption was measured. Percent biodegradation is based on theoretical oxygen demand.
Source	:	Exxon Biomedical Sciences, Inc.

29.07.1998 (63)

Type	:	aerobic
Inoculum	:	activated sludge, adapted
Concentration	:	3mg/l related to Test substance related to
Contact time	:	
Degradation	:	> 90 - % after 5 day
Result	:	
Deg. Product	:	
Method	:	other: 19-day Die-Away Test (US Environmental Protection Agency)
Year	:	1979
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Purity: not specified The semi-continuous activated sludge (SCAS) test simulates sewage treatment plant conditions. SCAS test systems that had been operated for 3 weeks were used to begin the die-away test. Primary biodegradation was determined by sample extraction and GC analysis of the parent compound.
Source	:	Exxon Biomedical Sciences, Inc.

28.07.1998 (111)

Type	:	aerobic
Inoculum	:	other: River Water
Concentration	:	1mg/l related to Test substance related to
Contact time	:	
Degradation	:	> 95 - % after 12 day
Result	:	
Kinetic of test substance	:	2 day = 20 - % 6 day = 46 - % - % - % - %
Deg. Product	:	
Method	:	other: Primary Test
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Exxon Biomedical Sciences, Inc.

30.07.1998 (16)

Type : aerobic
Inoculum : activated sludge, adapted
Contact time :
Degradation : = 67.8 - % after 1 day
Result :
Deg. Product :
Method : other: Semi-Continuous Activated Sludge (SCAS) Test
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Purity: not specified
The semi-continuous activated sludge test simulates sewage treatment plant conditions. Primary biodegradation was determined by sample extraction and GC analysis of the parent compound. The daily addition of test material was 1 mg/l during the first week of operation and 3 mg/l during the second and third weeks of operation.
Source : Exxon Biomedical Sciences, Inc.
28.07.1998 (111)

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 20mg/l related to Test substance
related to
Contact time :
Degradation : = 62 - % after 28 day
Result :
Kinetic of test substance : 7 day = 5 - %

9 day = 12 - %
14 day = 41 - %
21 day = 57 - %
28 day = 62 - %
Deg. Product :
Method : other: Shake Flask CO2 Evolution Test
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Purity: not specified
Ultimate biodegradation to carbon dioxide was measured by shake flask CO2 evolution test method. The half-life was calculated as 5.31 days. The lag phase was 7.1 days. The rate constant was 0.131 days-1.
Source : Exxon Biomedical Sciences, Inc.
28.07.1998 (140)

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 20mg/l related to Test substance
related to
Contact time :
Degradation : > 99 - % after 28 day
Result :
Deg. Product :
Method : other: Shake Flask CO2 Evolution Test
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : The parent compound was extracted from the test systems and analyzed by GC on day 28 only to determine primary biodegradation.

Source : Exxon Biomedical Sciences, Inc.
28.07.1998 (140)

Type : aerobic
Inoculum : other: Freshwater and sediment (see remark)
Contact time :
Degradation : ca. 1 - 8 % after 28 day
Result :
Deg. Product :
Method : other: respirometer
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : The freshwater/sediment inoculum was obtained from Little Dixie Lake, Columbia, Missouri, USA. The water/sediment ratio was 9:1 (wt:wt). The test compound was 14C-carbonyl labelled DINP. Biodegradation was monitored and measured by trapping and counting 14CO2 evolution. Biodegradation of DINP was measured with a range of test substance concentrations (0.0197 to 10.0 mg/L) and temperatures (12, 22, and 28C), as well as with the use of an acclimated and non acclimated inoculum.
Source : Exxon Biomedical Sciences, Inc.
30.07.1998 (93)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species : other: Arca zebra (Mollusca)
Exposure period : 1 day at 26.5 degree C
Concentration : 61µg/l
BCF : = 4.7 -
Elimination : yes
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : Steady-state BCF is based on the total radioactivity determined in muscle (foot) and water and does not distinguish parent compound from metabolites.
Source : Exxon Biomedical Sciences, Inc.
01.02.1999 (133)

Species : other: Diplora strigosa (Coelenterata)
Exposure period : 1 day at 26.5 degree C
Concentration : 61µg/l
Elimination : yes
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : Values reported are based on the total radioactivity determined for protein content in whole-tissue (and associated zooxanthellae) and water. The BCF immediately following exposure = 0.46; The values do not distinguish parent compound from metabolites. Authors state that DINP was poorly accummulated in the coral tissue, and

approximately 50% was eliminated during the first 4 days after transfer to clean seawater.

Source : Exxon Biomedical Sciences, Inc.
01.02.1999 (133)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Cyprinodon variegatus (Fish, estuary, marine)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC0	:	= .52 -
Method	:	other: US EPA-660/3-75-009
Year	:	1975
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	No toxicity was observed at the concentration reported. This was the maximum attainable test concentration due to the limits of solubility in the test waters. The LC0 was recalculated using all measured values (Adams et al., 1995). The original LC0 was cited as LC50 > 0.52 mg/l in a report submitted to CMA.
Source	:	Exxon Biomedical Sciences, Inc.

29.07.1998 (11) (135)

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC0	:	= .16 -
Method	:	other: US EPA-660/3-75-009
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	No toxicity was observed at the concentration reported. This was the maximum attainable test concentration due to the limits of solubility in the test waters. The LC0 was recalculated using all measrued values (Adams et al., 1995). The original LC0 was cited as LC50 > 0.16 mg/l in a report submitted to CMA.
Source	:	Exxon Biomedical Sciences, Inc.

31.07.1998 (11) (48)

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC0	:	= .19 -
Method	:	other: US EPA-660/3-75-009
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	No toxicity was observed at the concentration reported. This was the maximum attainable test concentraion due to the limits of solubility in the test waters. The LC0 was recalculated using all measured values (Adams et al., 1995). Th original LC0 was cited as LC50 > 0.19 mg/l in a report submitted to CMA.
Source	:	Exxon Biomedical Sciences, Inc.

28.07.1998 (11) (50)

Type	:	semistatic
Species	:	Ictalurus punctatus (Fish, fresh water)
Exposure period	:	
Unit	:	mg/l
Analytical monitoring	:	no
EC50	:	= .42 -
Method	:	other: details in referenced article
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Exposed egg stage (2-6 hr post-spawn) through 4 days post-hatch. The "EC50" was based on mortality plus teratogenesis. A stock solution (emulsion) was prepared by mixing DINP:acetone (100:4 ratio) with water in a blender. The stock solution was diluted to prepare the exposure treatments (100, 10, 1, 0.1, 0.01 mg/l DINP). These results are based on exposure to an emulsion, prepared at levels far above the water solubility of DINP, and are therefore of no value for hazard or risk assessment purposes.
Source	:	Exxon Biomedical Sciences, Inc.
Reliability	:	(3) invalid

31.07.1998 (26)

Type	:	semistatic
Species	:	Lepomis microlophus (Fish, fresh water)
Exposure period	:	
Unit	:	mg/l
Analytical monitoring	:	no
EC50	:	= 4.67 -
Method	:	other: details in referenced article
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Exposed egg stage (2-6 hr post-spawn) through 4 days post-hatch. The "EC50" was based on mortality plus teratogenesis. A stock solution (emulsion) was prepared by mixing DINP:acetone (100:4 ratio) with water in a blender. The stock solution was diluted to prepare the exposure treatments (100, 10, 1, 0.1, 0.01 mg/l DINP). These results are based on exposure to an emulsion, prepared at levels far above the water solubility of DINP, and are therefore of no value for hazard or risk assessment purposes.
Source	:	Exxon Biomedical Sciences, Inc.
Reliability	:	(3) invalid

31.07.1998 (26)

Type	:	semistatic
Species	:	other: amphibian: Bufo fowleri (toad)
Exposure period	:	
Unit	:	mg/l
Analytical monitoring	:	no
EC50	:	= 2.95 -
Method	:	other: details in referenced article
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Exposed egg stage (2-6 hr post-spawn) through 4 days post-hatch. The "EC50" was based on mortality plus teratogenesis. A stock solution (emulsion) was prepared by mixing DINP:acetone (100:4 ratio) with water in a blender. The stock solution was diluted to prepare the exposure treatments (100, 10, 1, 0.1, 0.01 mg/l DINP). These results

are based on exposure to an emulsion, prepared at levels far above the water solubility of DINP, and are therefore of no value for hazard or risk assessment purposes.

Source : Exxon Biomedical Sciences, Inc.
Reliability : (3) invalid
31.07.1998 (26)

Type : semistatic
Species : other: amphibian: Rana pipiens (frog)
Exposure period :
Unit : mg/l
Analytical monitoring : no
EC50 : = 3.63 -
Method : other: details in referenced article
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Exposed egg stage (2-6 hr post-spawn) through 4 days post-hatch. The "EC50" was based on mortality plus teratogenesis. A stock solution (emulsion) was prepared by mixing DINP:acetone (100:4 ratio) with water in a blender. The stock solution was diluted to prepare the exposure treatments (100, 10, 1, 0.1, 0.01 mg/l DINP). These results are based on exposure to an emulsion, prepared at levels far above the water solubility of DINP, and are therefore of no value for hazard or risk assessment purposes.
Source : Exxon Biomedical Sciences, Inc.
Reliability : (3) invalid
31.07.1998 (26)

Type : static
Species : Lepomis macrochirus (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : yes
LC0 : = .14 -
Method : other: US EPA-660/3-75-009
Year : 1975
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : No toxicity was observed at the concentration reported. This was the maximum attainable test concentration due to the limits of solubility in the test waters.
The LC0 was recalculated using all measured values (Adams et al., 1995). The original LC0 was cited as LC50 > 0.17 mg/l in a report submitted to CMA.
Source : Exxon Biomedical Sciences, Inc.
28.07.1998 (11) (49)

Type : static
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : yes
LC0 : = .1 -
Method : other: US EPA-660/3-75-009
Year : 1975
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : No toxicity was observed at the concentration reported. This was the maximum attainable test concentration due to the limits of solubility in the test waters.

The LC0 was recalculated using all measured values (Adams et al., 1995). The origianl LC0 was cited as LC50 > 0.14 mg/l in a report submitted to CMA.

Source : Exxon Biomedical Sciences, Inc.
09.02.1999 (11) (47)

Type : static
Species : other: amphibian: Rana arvalis (Moorfrog)
Exposure period : 26 day
Unit :
Analytical monitoring : yes
Method : other
Year : 2000
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : Egg hatchability and larval survival / development examined in presence of test substance in two types of sediment. Fine sediment (mostly degraded organic material) and coarse sediment (freshly deposited material). Exposure temperature = 10°C. Embryos were field collected and held until used.

Three treatment concentration of 1000, 300, and 100 mg DINP/kg dwt together with solvent and unspiked sediment controls. Five replicates per treatment.

DINP showed no significant effect on the hatching frequency, median hatching time, or larval mortality at any of the tested concentrations when compared to the control groups.

Source : ExxonMobil Biomedical Sciences, Inc.
Reliability : (2) valid with restrictions
12.06.2001 (134)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : no
EC0 : = 1 -
Method : OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year : 1984
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Tested a nominal concentration of 1 mg/l DINP with a dispersant concentration (Castor Oil 40 Ethoxylate) of 10mg/l. No observed effects at the tested concentration.

Source : Exxon Biomedical Sciences, Inc.
08.06.2001 (30)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : yes
EC0 : = .06 -
Method : other: US EPA-660/3-75-009
Year : 1975
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : No toxicity was observed at the concentration reported. This was the maximum attainable test concentration due to the limits of solubility in the test waters. The EC0 was recalculated using all measured values (Adams et al., 1995). The original EC0 was cited as EC50 > 0.086 mg/l in a report submitted to CMA.
Source : Exxon Biomedical Sciences, Inc.
28.07.1998 (11) (136)

Type :
Species : Mysidopsis bahia (Crustacea)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : yes
LC0 : = .39 -
Method : other: US EPA-660/3-75-009
Year : 1975
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : No toxicity was observed at the concentration reported. This was the maximum attainable test concentration due to the limits of solubility in the test waters. The LC0 was recalculated using all measured values (Adams et al., 1995). The original LC0 was cited as LC50 > 0.77 mg/l in a report submitted to CMA.
Source : Exxon Biomedical Sciences, Inc.
28.07.1998 (11) (51)

Type : other: sediment
Species : other: Chironomus tentans
Exposure period : 10 day
Unit : mg/kg soil dw
Analytical monitoring : yes
NOEC : 2680 -
Method : other: EPA/600/R-94/024
Year : 1994
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Endpoints: Survival and growth
Tested at nominal concentration of 3000 mg/kg - dw of DINP. No effect observed on survival or growth during the 10-day exposure.
Source : ExxonMobil Biomedical Sciences, Inc
Reliability : (2) valid with restrictions
12.06.2001 (36)

Type : other: sediment
Species : other: Hyalella azteca
Exposure period : 10 day
Unit : mg/kg soil dw
Analytical monitoring : yes
NOEC : 2900 -
Method : other: EPA/600/R-94/024
Year : 1994
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Endpoints: Survival and growth
Source : ExxonMobil Biomedical Sciences, Inc.
Reliability : (2) valid with restrictions
12.06.2001 (36)

Type :
Species : other: Paratanytarsus parthenogenica

Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC0	:	= .08 -
Method	:	other: US EPA-660/3-75-009
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	No toxicity was observed at the concentration reported. This was the maximum attainable test concentration due to the limits of solubility in the test waters. The LC0 was recalculated using all measured values (Adams et al., 1995). The original LC0 was cited as LC50 > 0.12 mg/l in a report submitted to CMA.
Source	:	Exxon Biomedical Sciences, Inc.

28.07.1998 (11) (52)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	other: cell number
Exposure period	:	120 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
EC0	:	= 1.8 -
Method	:	other: US EPA-600/9-78-018
Year	:	1978
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	No toxicity was observed at the concentration reported. This was the maximum attainable test concentration due to the limits of solubility in the test waters. The EC0 was recalculated using all measured values (Adams et al., 1995). The original EC0 was cited as EC50 > 2.8 mg/l in a report submitted to CMA. The exposure duration (96 hours) for the test as cited in Adams et al. is incorrect. The CMA report cites the correct duration as 120 hours.
Source	:	Exxon Biomedical Sciences, Inc.

28.07.1998 (11) (53)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type	:	aquatic
Species	:	activated sludge of a predominantly domestic sewage
Exposure period	:	30 minute(s)
Unit	:	mg/l
Analytical monitoring	:	yes
EC0	:	= 83.9 -
Method	:	OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A stock solution was prepared using a 1:10 ratio of test material:Tween 20 dispersant.
Source	:	Exxon Biomedical Sciences, Inc.

28.07.1998 (69)

Type	:	aquatic
Species	:	activated sludge, domestic
Exposure period	:	30 minute(s)
Unit	:	mg/l
Analytical monitoring	:	
EC0	:	= 83 -
Method	:	OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year	:	1984
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A stock solution was perpared using a 1:10 ratio of test substance: Tween 20 dispersant.
Source	:	ExxonMobil Biomedical Sciences, Inc.

12.06.2001 (70)

Type	:	aquatic
Species	:	Photobacterium phosphoreum (Bacteria)
Exposure period	:	15 minute(s)
Unit	:	mg/l
Analytical monitoring	:	
EC0	:	= 83 -
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A stock solution was prepared using a 1:10 ratio of test substance: Tween 20 dispersant.
Source	:	ExxonMobil Biomedical Sciences, Inc.

12.06.2001 (71)

Type	:	aquatic
Species	:	Photobacterium phosphoreum (Bacteria)
Exposure period	:	15 minute(s)
Unit	:	mg/l
Analytical monitoring	:	yes
EC0	:	= 83.9 -
Method	:	other: Microtox Toxicity Test
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Stock solution was prepared using a 1:10 ratio of test material:Tween 20 dispersant.
Source	:	Exxon Biomedical Sciences, Inc.

28.07.1998 (69)

4.5.1 CHRONIC TOXICITY TO FISH

Species	:	Oryzias latipes (Fish, fresh water)
Endpoint	:	
Exposure period	:	284 day
Unit	:	
Analytical monitoring	:	yes
Method	:	
Year	:	2001
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Test substance was tested in a multi-generation dietary exposure protocol to evaluate reproductive and developmental effects in the Japanes Medaka. Test substance was spiked via an acetone solution into a fish flake food at 20µg/g. Fish were fed at a daily rate of 5% body weight / day.

Fo and F1 generation adults were reared through sexual maturation and ovipositor (140 days-post-hatch). Test ended with F2 generation prior to sexual maturation.

Effects were evaluated using population, individual, and biochemical parameters including: survival, sex ratio, fecundity, development, growth, gonadal-somatic index, histopathology,
testosterone metabolism, EROD activity, and vitellogenin production.

Results indicated that egg production was similar among all treatment groups. F1 and F2 generation embryos showed normal development except for transient change in red blood cell pigmentation in the phthalate and acetone groups. There were no treatment-related alterations in survival, fecundity, or GSI and no histological lesions were observed.

There was no shift in male-to-female ratio and the phenotypic and histological gender classifications for both male and female fish were in agreement. Testosterone metabolism, EROD activity, and vitellogenin levels were not significantly different among treatment groups.

Source : ExxonMobil Biomedical Sciences, Inc.
Reliability : (1) valid without restriction
12.06.2001 (116)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species : Daphnia magna (Crustacea)
Endpoint : other: survival and reproduction
Exposure period : 21 day
Unit : mg/l
Analytical monitoring : yes
NOEC : = .034 -
Method : other: EG&G Bionomics chronic toxicity test
Year : 1982
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : The study was confounded by surface filming and suface entrapment of test organisms. The results after 21 days showed effects on survival and reproduction in comparison to the controls for the two high concentrations. However, these effects are attributed to physical effects associated with testing this hydrophobic liquid at concentrations well in excess of water solubility. Consequently, the results of this study are concluded not to be valid for toxicity assessment.
Source : Exxon Biomedical Sciences, Inc.
Reliability : (3) invalid
03.05.2001 (137)

Species : Daphnia magna (Crustacea)
Endpoint : other: survival, growth, and reproduction
Exposure period : 21 day
Unit : mg/l
Analytical monitoring : yes
NOEC : = 1 -
Method : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year : 1984
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : The endpoints measured were survival, growth, and reproduction. Tested at a nominal concentration of 1 mg/l with a dispersant concentration (Castor Oil 40

Ethoxylate) of 10 mg/l. Analyses of the stock solutions showed that the PAE concentration ranged from 100-110% of nominal (105% mean). Results showed that there was no difference between the exposure solution and the controls for all endpoints observed.

Source : Exxon Biomedical Sciences, Inc.
31.07.1998 (29)

Species : Daphnia magna (Crustacea)
Endpoint : other: survival, growth, and reproduction
Exposure period : 21 day
Unit : µg/l
Analytical monitoring : yes
NOEC : = 1.28 -
Method : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Tested the Water Accommodated Fraction of a nominal loading of 2 mg/l DINP. Results showed that there was no difference between the exposure solution and the controls for all endpoints observed.
Source : Exxon Biomedical Sciences, Inc.
01.06.2001 (62)

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

Type : artificial soil
Species : Eisenia fetida (Worm (Annelida), soil dwelling)
Endpoint : mortality
Exposure period : 14 day
Unit : mg/kg soil dw
LC0 : = 7996 -
Method : OECD Guide-line 207 "Earthworm, Acute Toxcity Test"
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Also tested in natural soil. The OECD 207 method was combined with US EPA -600/3-88-029 method. Measured test material concentrations in worms at test termination, following a 3 hour purge of gut. Results: = 134 (natural soil) and 145 (artificial soil) mg/kg wet weight.
Source : Exxon Biomedical Sciences, Inc.
26.04.2001 (65)

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

Species : Lolium perenne (Monocotyledon)
Endpoint : emergence
Exposure period : 5 day
Unit : mg/kg soil dw
NOEC : = 8268 -
Method : other: US EPA-600/3-88-029
Year : 1988
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Tested in both a sand/artificial soil mixture and a natural soil.

Source : Exxon Biomedical Science, Inc.
28.07.1998 (66)

Species : Lactuca sativa (Dicotyledon)
Endpoint : emergence
Exposure period : 5 day
Unit : mg/kg soil dw
NOEC : < 8267 -
Method : other: US EPA-600/3-88-029
Year : 1988
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Tested in both a sand/artificial soil mixture and a natural soil.

Source : Exxon Biomedical Sciences, Inc.
28.07.1998 (66)

Species : Lactuca sativa (Dicotyledon)
Endpoint : emergence
Exposure period : 5 day
Unit : mg/kg soil dw
NOEC : = 1049 -
LOEC : = 2778 -
Method : other: US EPA-600/3-88-029
Year : 1988
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Tested in both a sand/artificial soil mixture and a natural soil.

Source : Exxon Biomedical Sciences, Inc.
31.07.1998 (67)

Species : Lactuca sativa (Dicotyledon)
Endpoint : other: Emergence and growth
Exposure period : 28 day
Unit : mg/kg soil dw
NOEC : 1500 -
Method : OECD Guide-line 208 "Terrestrial Plants, Growth Test"
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Three concentrations tested 1500, 750, and 375 mg/kg. A natural soil control was also tested. Thirty replicates for each treatment and control. At end of exposure, number of germinated plants recorded. Plants were then cut at soil level and individual weighed.

Source : ExxonMobil Biomedical Sciences, Inc.
12.06.2001 (72)

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	30
Vehicle	:	no data
Value	:	> 10000 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	DINP was administered by gastric intubation to groups of 5 fasted rats. Dose levels: 34.6, 120, 417, 1450, 5000 and 10,000 mg/kg of body weight. A 14 day observation was used. No deaths occurred at any of the levels tested. Depressed, laboured respiration and oily-appearing fur were noted at levels of 5,000 mg/kg and above. Recovery occurred within three to seven days. Weight loss was observed at 10,000 mg/kg. No major necropsy findings were observed at any dose level.
Conclusion	:	The acute oral LD50 is greater than 10,000 mg/kg/day.

15.10.2001 (9)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Species	:	laboratory animal
Strain	:	other
Sex	:	male/female
Number of animals	:	30
Vehicle	:	other: air control
Exposure time	:	6 hour(s)
Value	:	> .067 - mg/l
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Wistar Rats, Swiss albino Mice, Harley Guinea Pigs
Remark	:	No deaths, observable reactions or pathologic alterations were seen. The test concentration in this study was very low due to the limited volatility of DINP. DINP is unlikely to be hazardous by inhalation due to its low volatility. Wistar Rats, Swiss albino Mice, Harley Guinea Pigs (n = 5 for control; n = 10 for treatment) were exposed to a nominal vapor concentration of 0.067 mg/l for 6 hours. A 14 day observation period was used.
Conclusion	:	The acute inhalation LC50 (6 hours) is greater than 0.067 mg/l.

20.04.2001 (10)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	16

Vehicle	:	no data
Value	:	> 3160 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A single 24-hour application of DINP was applied at concentrations of 50, 200, 794 and 3160 mg/kg to the abraded rabbit skin under occlusive covering (n = 4). A 14 day observation period was used. There were no deaths and no evidence of systemic toxicity at any dose level.
Conclusion	:	The acute dermal LD50 is greater than 3160 mg/kg.

18.04.2001 (7)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	.5 undiluted
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	6
PDII	:	.08
Result	:	not irritating
EC classification	:	not irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1992
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Very slight erythema (score 1) was observed in one animal at 1 hour and in another animal at 24 hours. All animals were free of erythema, oedema, or other supplemental dermal findings during the remainder of the study. Clincal signs were not observed during the test period.

20.04.2001 (122)

Species	:	human
Concentration	:	100 %
Exposure	:	Occlusive
Exposure time	:	42 day
Number of animals	:	104
PDII	:	
Result	:	not irritating
EC classification	:	not irritating
Method	:	other: single 24 hour application
Year	:	1999
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	DINP was administered to human volunteers via a single 24-hour occluded patch application. Evaluations were made at 30 minutes and 24 hours after patch removal. No dermal responses were observed. The group mean irritation score was 0.00

20.04.2001 (57) (103)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	undiluted
Dose	:	.1 ml
Exposure Time	:	
Comment	:	no data
Number of animals	:	
Result	:	slightly irritating
EC classification	:	not irritating
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	0.1 ml of undiluted DINP was applied into the conjunctival sac of the left eye of six rabbits. Scoring was carried out after 1, 4, 24, 48 and 72 hours and at 4 and 7 days. Irritation was confined to the conjunctivae and generally consisted of marked redness and slight discharge at one and four hours (score of 3), and slight redness (moderate in one eye) only at 24 hours (score of 1). By 48 or 72 hours, the irritation had completely subsided in all eyes.

18.04.2001 (8)

5.3 SENSITIZATION

Type	:	Buehler Test
Species	:	guinea pig
Concentration	:	Induction .4 undiluted occlusive epicutaneous Challenge 5 % occlusive epicutaneous Challenge 5 % occlusive epicutaneous
Number of animals	:	40
Vehicle	:	Peanut Oil
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	OECD Guide-line 406 "Skin Sensitization"
Year	:	1981
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A Buehler test was carried out on forty female guinea pigs (20 control and 20 treated) with (DINP). The substance was administered neat (0.4 ml) at day 0, 7, 14 during 6 hours under occlusive bandaging, followed by a challenge application of DINP at 5% in peanut oil at day 28 and by a rechallenge at the same concentration at day 35. A primary irritation test was conducted first to determine the concentration of the test material to be used in the two phases of dosing. As DINP was not irritating, a concentration of 5.0% (w/w) was applied topically to the clipped area. Topical application of DINP during the induction of the treated group animals produced erythema ranging from very slight to well-defined in all twenty animals. Oedema was also noted during induction in all treated animals and ranged from very slight to slight. No erythema or oedema was observed at the first challenge in the treated (20 animals) or negative control (10 animals group. However, reactions were observed during rechallenge; erythema was observed at day 36 on 10 treated animals (score 1); at day 37 on 4 animals (score 1); and 3 animals (score 2). Oedema was noted at day 37 in 1 of the treated animals (score 1). Erythema (score 1) was also observed at day 37 in 4 animals among 10 control animals.

18.04.2001 (44)

Type	:	Buehler Test
Species	:	guinea pig

Concentration	:	Induction .5 undiluted occlusive epicutaneous Challenge .5 undiluted occlusive epicutaneous Challenge .5 undiluted occlusive epicutaneous
Number of animals	:	40
Vehicle	:	no data
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	other: Directive 92/69/EEC, B.6
Year	:	1992
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A Buehler test was carried out on forty female guinea pigs (20 control and 20 treated animals) with DINP. The substance was applied neat (0.5 ml) for induction at day 1-8-15 during 6 hours under occlusive bandaging and for challenge at day 29. No evidence of skin sensitization was observed in any of the treated animals. This test was conducted in conformity with GLP procedures and with EEC Method B6.

01.06.2001 (45)

Type	:	Patch-Test
Species	:	human
Concentration	:	Induction .2 undiluted Challenge .2 undiluted Challenge .2 undiluted
Number of animals	:	104
Vehicle	:	other: undiluted material
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	other: modified Draize procedure
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A RIPT (Repeated Insult Patch Test) was carried out with 28 subjects in the pilot study and 76 subjects in the definitive study using (DINP). The substance was administered neat (0.2 ml). Induction applications were made three times per week for three successive weeks. A challenge application was made after a 10 to 17-day rest period. None of the volunteers responded to the challenge dose, and the test material was judged to be non-sensitizing.

20.04.2001 (104) (126)

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male/female
Strain	:	other: Charles River Caesarean-derived strain
Route of admin.	:	oral feed
Exposure period	:	3 months
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	50, 150 and 500 mg/kg/day
Control group	:	yes
NOAEL	:	= 150 - mg/kg bw
LOAEL	:	= 500 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	10 rats/sex/group were fed 50, 150 and 500 mg/kg/day DINP

for 3 months. Criteria for evaluation of a compound effect were physical appearance and behavior, survival, growth and food consumption, clinical laboratory results, organ weight data, and gross and microscopic examination. All animals survived and there was no gross evidence of toxicologic effects. Treatment-related effects which were seen only in high dose animals included ELEVATED LIVER WEIGHTS in both sexes and ELEVATED KIDNEY WEIGHTS in the females. Additionally, HEPATOCYTIC HYPERTROPHY was seen in high dose males and females. The absolute and relative testis weights were comparable among control and treated groups. No remarkable microscopic changes were observed in ovaries and testes preserved in 10% neutral buffered formalin.

Conclusion : The no effect level (NOEL) for all effects was 150 mg/kg/day. However, the effects at the 500 mg/kg/day level, predominantly weight changes in the liver and kidney, were associated with peroxisomal proliferation, a mechanism which has no clinical relevance to humans. Thus, the no observed adverse effect level (NOAEL) was 500 mg/kg/day.

26.04.2001 (144)

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : oral feed
Exposure period : 13 weeks
Frequency of treatment : daily
Post obs. period : none
Doses : 0.1, 0.3, 0.6, 1.0, and 2.0 % (approx. 77, 227, 460, 767 and 1554 mg/kg/day)
Control group : yes
NOAEL : ca. 77 - mg/kg bw
LOAEL : ca. 227 - mg/kg bw
Method : other: not specified
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : There were no deaths prior to study termination. A significant depression in food consumption and body weight gain was noted in the high dose group. No significant hematologic changes were observed. Clinical chemistry values for triglycerides showed a dose-related decrease while albumin-globulin ratios showed a dose-related elevation. Absolute and relative kidney and liver weights of various treated groups (equal to or greater than 3000 ppm) were increased as compared to controls. Kidney lesions (nephrotic and regenerative changes) were found only in males treated with at least 3000 ppm DINP. A dose-related diffuse cytoplasmic eosinophilic hypertrophy of liver hepatocytes was observed in all treatment groups. Electron microscopic examination of the liver showed a dose-related proliferation of peroxisomes and smooth endoplasmic reticulum of groups exposed to at least 6000 ppm.

Conclusion : High doses of DINP produced liver and kidney changes in rats. The no observed effect level (NOEL) for all effects was 1000 ppm (approximately 77 mg/kg/day). However, liver effects seen at higher levels were the consequence of peroxisomal proliferation and without clinical relevance to humans.

23.04.2001 (24) (143)

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : oral feed
Exposure period : 21 days

Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	0.6, 1.2 and 2.5% (approx. 600, 1200 and 2200 mg/kg/day)
Control group	:	yes
NOAEL	:	ca. 600 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	yes
Test substance	:	other TS: mixture of commercial DINPs
Remark	:	All animals survived and there was no gross evidence of toxicologic effects. Treatment-related effects at the 0.6% dose included DECREASED SERUM CHOLESTEROL LEVELS, INCREASED LAURIC ACID 11- and 12-HYDROXYLASE LEVELS, INCREASED TOTAL HEPATIC PROTEIN LEVELS AND ELEVATED LIVER WEIGHTS. DECREASED BODY WEIGHT GAIN was seen in groups exposed to 1.2% and above. PEROXISOME PROLIFERATION was seen only in high dose males and females. These changes at the 0.6% dose are believed to be physiologically adaptive, and therefore not adverse or biologically significant. Testicular weights were unaffected at all doses.
Conclusion	:	The NOAEL from this study is approximately 600 mg/kg/day.

01.06.2001 (22)

Species	:	rat
Sex	:	male
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	1 week
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	2% (approx. 1700 mg/kg/day)
Control group	:	yes, concurrent no treatment
NOAEL	:	ca. 1700 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Treatment-related effects included DECREASED SERUM CHOLESTEROL AND TRIGLYCERIDE LEVELS and ELEVATED LIVER WEIGHTS. At necropsy, LIVER CONGESTION was seen in 3/8 male rats. No histological changes were observed.
Conclusion	:	These changes are not considered to be relevant to humans. Therefore, the NOAEL from this study is greater than 1700 mg/kg/day.

20.04.2001 (115)

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	13 weeks
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	0.3 and 1.0% (approximately 227 and 460 mg/kg/day)
Control group	:	yes
NOAEL	:	ca. 460 - mg/kg bw
Method	:	other: not specified
Year	:	1982
GLP	:	yes

Test substance	:	as prescribed by 1.1 - 1.4
Method	:	In a 13-week feeding study, groups of 15 Sprague Dawley rats of each sex were fed diets containing 0-0.3-1.0% which correspond respectively to 201-690 mg/kg/day in males and to 251-880 mg/kg/day in females
Remark	:	There was one death in the 1% group during the final week. There was no gross evidence of toxicologic effects. Treatment-related effects included decreased serum triglycerides and decreased means for all RBC parameters, suggestive of mild anemia. Elevated liver and kidney weights were observed in low dose females and high dose males and females. Additionally, alkaline phosphatase levels were increased in high dose animals. Few in-life observations were noted during the study. Mean body weights and food consumption showed normal patterns in all groups until week 12 of the study. At that time, treated animals showed a sharp decrease in body weight means which was statistically significant. This might have been related to a watering system uncoupling during the last week.
Conclusion	:	As the highest treatment level was not associated with effects which were clinically relevant to humans, the NOAEL was greater than 460 mg/kg/day.

23.04.2001 (142)

Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	oral feed
Exposure period	:	13 weeks
Frequency of treatment	:	Continuous
Post obs. period	:	no data
Doses	:	1,500, 4,000, 10,000, 20,000 ppm
Control group	:	yes, concurrent no treatment
NOAEL	:	= 4000 - ppm
Method	:	other
Year	:	1992
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	DINP was administered to B6C3F1 mice in the diet for 13 weeks. Ten mice/sex/group received test material at dose levels of 1,500-4,000-10,000 and 20,000 ppm (about 365-972-2,600-5,770 mg/kg/d)(groups 2 to 5 respectively). An additional group of 10 mice/sex/group received the basal diet only and served as the negative control group (group 1). To evaluate the hepatocellular proliferation and peroxisomal proliferation, additional corresponding groups of 15 mice/sex/group were evaluated 3, 30 and 90 days after study. Criteria evaluated in treated animals included survival, food consumption body weight, ophthalmology, clinical pathology, organ weight, gross pathology and microscopic pathology. Tissues were preserved in 10% neural buffered formalin and embedded in paraffin. Assessment of peroxisomal potential was also made in additional animals (biochemical parameters and microscopy).
Result	:	Enlarged livers were observed in male rats given diets containing 4,000 ppm and higher, and in females given diets containing 10,000 ppm and higher. Pale areas were sometimes seen in males from 10,000 ppm and in females at 20,000 ppm. Granular/pitted/rough kidneys were noted in some group 5 animals. Small uteri were observed in group 5 females and thickening of the uterine wall was noted in 1/10 female at 1,500 and 2/8 at 10,000 ppm. In a satellite study, the same liver findings were observed in group 3 through 5 animals and in positive controls and only one small uterus was noted for one positive control female.
Conclusion	:	A NOEL of 1,500 ppm (about 365 mg/kg/d) was determined for this 13 week study, due to the effects on the liver at 4,000 ppm (enlarged liver and increases of absolute and relative liver weight). However, these effects were the consequence of a peroxisomal proliferation process and not clinically relevant to humans. A NOAEL of 4,000 ppm (approximately 972

mg/kg/day) was determined for reproductive organ effects based on decreased absolute testis/epididymis weights in the 10000 ppm group.

26.04.2001 (83)

Species	:	rabbit
Sex	:	male/female
Strain	:	New Zealand white
Route of admin.	:	dermal
Exposure period	:	6 weeks
Frequency of treatment	:	daily, 5 days/week
Post obs. period	:	
Doses	:	0.5 and 2.5 ml/kg
Control group	:	yes
NOAEL	:	> 2.5 -
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Four animals were tested in each group. Applications were made once daily, five days a week for a total of 30 exposures at dosage levels of 0.5 and 2.5 ml/kg. Applications were on abraded and intact skin. Criteria used to evaluate compound effect were physical appearance, behavior, body weight, survival, dermal irritation, clinical laboratory studies, and gross and microscopic pathology. There was no evidence of systemic toxicity from repeated dermal exposure to DINP. At the 2.5 ml/kg dose level, slight to moderate erythema was seen (abraded skin only).

18.03.1996 (125)

Species	:	dog
Sex	:	male/female
Strain	:	Beagle
Route of admin.	:	oral feed
Exposure period	:	13 weeks
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	0.125, 0.5, and 2.0% (increased to 4.0% at week 9) (approx. 37, 160 and 2000 mg/kg/day)
Control group	:	yes, concurrent no treatment
NOAEL	:	ca. 160 - mg/kg bw
LOAEL	:	ca. 2000 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	4 dogs/sex/group were fed DINP at dietary levels of 0.125, 0.5 and 2% for 13 weeks. The 2% dose was increased to 4% for weeks 9 to 13. Criteria for evaluation of a compound effect were physical appearance and behavior, survival, growth and food consumption, clinical laboratory results, organ weight data, and gross and microscopic pathology. All animals survived and there was no gross evidence of toxicologic effects. Treatment-related effects which were seen only in high dose animals included ELEVATED LIVER WEIGHTS and ENZYMES (SG-OT, SG-PT), DECREASED TOTAL HEPATIC PROTEIN AND ALBUMIN LEVELS. Microscopic liver and kidney effects were also observed.

18.04.2001 (1)

Species	:	monkey
Sex	:	male
Strain	:	other
Route of admin.	:	gavage
Exposure period	:	14 days
Frequency of treatment	:	daily
Post obs. period	:	1 day
Doses	:	500 mg/kg/day
Control group	:	yes, concurrent vehicle
NOAEL	:	500 - mg/kg
LOAEL	:	> 500 - mg/kg
Method	:	
Year	:	1997
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A portion of the study was conducted under GLPs.
Result	:	No treatment related mortality or adverse toxicological, pharmacological or clinical signs were noted in any of the monkeys.
Reliability	:	(2) valid with restrictions

23.04.2001 (123)

Species	:	monkey
Sex	:	male/female
Strain	:	Marmoset
Route of admin.	:	gavage
Exposure period	:	13 weeks
Frequency of treatment	:	daily
Post obs. period	:	5 weeks (17 for parameters for hematology and 18 parameters for biochemistry)
Doses	:	0 100, 500 & 2,500 mg/kg/day
Control group	:	yes
NOAEL	:	= 500 - mg/kg bw
Method	:	other
Year	:	1998
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	In a marmoset monkey study, four groups per sex/group were administered DINP daily by gavage at dose levels of 0- 100- 500- 2,500 mg/kg/day for a period of 13 weeks after a 3-week acclimatization period. An additional group was treated with 500 mg/kg/d clofibrate to act as a reference control. This study was performed according to OECD TG and conducted in accordance with GLP. Animals were examined daily for clinical symptoms and food consumption and weighed weekly. An ophthalmoscopic examination was performed before the treatment and at week 12. Blood samples were obtained and analyzed before treatment and during weeks 6 and 13 (17 parameters for hematology and 18 parameters for biochemistry). Additional blood samples were obtained before the study and at week 12 for assessing hormonal parameters: Oestradiol and testosterone. Overnight urine was collected and analyzed before the study and during week 5 and week 12 of the treatment. At the end of the treatment period, animals were sacrificed and examined for gross pathologies, organs were weighed, liver samples (minimum 5g) were obtained as soon as possible after weighting, frozen immediately in liquid nitrogen and embedded in paraffin wax. Most tissues were preserved in 10 % neutral buffered formalin except eyes (preserved in Davinson's fluid), testes and epididymides (preserved in Bouin's fluid).
Remark	:	Body weight losses or low body weight gains were observed for males and

females at 2,500 mg/kg/day DINP. There were no treatment-related changes in biochemical parameters (including triglycerides and cholesterol) or in hormonal concentrations assessed. No histological findings were considered to be treatment-related. No changes in weights or macroscopic / microscopic findings were observed for testes.

Conclusion : In conclusion, at the high dose of 2,500 mg/kg/day DINP, only elicited minor changes which were: decreases of body weight and body weight gain. Therefore a conservative NOAEL of 500 mg/kg day can be assumed for systemic toxicity.

23.04.2001 (80) (87)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella strains TA98, 100, 1535, 1537 and 1538
Concentration : 0.5 to 5000 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year : 1983
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
01.06.2001 (102) (106)

Type : Ames test
System of testing : Salmonella strains TA98, TA100, TA1535, and TA1537
Concentration : up to 10 mg/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: Ames B.N. et al. Mutat. Res. 31:347-364.
Year : 1975
GLP : yes
Test substance : other TS: mixture of commercial DINPs
01.06.2001 (154)

Type : Ames test
System of testing : Salmonella strains TA98, TA100, TA1535 TA1537 and TA1538
Concentration : 0.1 to 10 ul/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: Ames BN et al. Mutat. Res. 31:347-364
Year : 1975
GLP : yes
Test substance : other TS: mixture of commercial DINPs
01.06.2001 (127)

Type : Cytogenetic assay
System of testing : Chinese hamster ovary cells
Concentration : 5 to 160 ug/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 473 "Genetic Toxicology: In vitro Mammalian Cytogenetic Test"
Year : 1983
GLP : yes

Test substance : as prescribed by 1.1 - 1.4
01.06.2001 (88) (102)

Type : Mouse lymphoma assay
System of testing : forward mutation assay, cell line L5178Y
Concentration : 500 - 8000 nl/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: Clive and Spector. Mutat. Res. 31:17-29.
Year : 1975
GLP : yes
Test substance : other TS: mixture of commercial DINPs
01.06.2001 (19) (108)

Type : Mouse lymphoma assay
System of testing : forward mutation assay, cell line L5178Y
Concentration : 7.5 - 100 ul/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: modication of Clive and Spector. Mutat. Res. 31:17-29.
Year : 1975
GLP : yes
Test substance : other TS: mixture of commercial DINPs
01.06.2001 (61)

Type : Unscheduled DNA synthesis
System of testing : rat primary hepatocytes
Concentration : 0, 0.625, 1.25, 2.5, 5.0 or 10.0 ul/ml
Cycotoxic conc. :
Metabolic activation : without
Result : negative
Method : other: based on William G.M. Cancer Res. 37:1845-1851.
Year : 1977
GLP : yes
Test substance : other TS: mixture of commercial DINPs
01.06.2001 (58)

Type : other: cell transformation assay
System of testing : BALB/C 3T3 cells
Concentration : 0.0326, 0.098, 0.326, 0.978 or 3.26 mg/l
Cycotoxic conc. :
Metabolic activation : without
Result : negative
Method : other: Kakunaga T. Int. J. Cancer 12:463-473
Year : 1973
GLP : yes
Test substance : other TS: mixture of commercial DINPs
01.06.2001 (20) (59)

Type : other: cell transformation assay
System of testing : BALB/C 3T3 cells
Concentration : 125, 398, 1250, 2500 and 3750 nl/ml
Cycotoxic conc. :
Metabolic activation : without
Result : negative
Method : other: adapted from Kakunaga T. Int. J. Cancer 12:463-473
Year : 1973
GLP : yes
Test substance : other TS: mixture of commercial DINPs
01.06.2001 (56)

Type : other: cell transformation assay
System of testing : BALB/C 3T3 cells
Concentration : 0.03, 0.1, 0.3 and 1.0 ul/ml
Cycotoxic conc. :
Metabolic activation : without
Result : negative
Method : other: modification of Schechtman and Kouri. In: Progress in Genetic Toxicology. D.Scott et al, eds. Elsevier/North Holland Biomedical Press, NY. pp.307-316.
Year : 1977
GLP : yes
Test substance : other TS: mixture of commercial DINPs
Remark : Test substance purity >99.9%.
01.06.2001 (5)

Type : other: cell transformation assay
System of testing : BALB/C 3T3 cells
Concentration : 0.1, 0.3 or 1.0 ul/ml
Cycotoxic conc. :
Metabolic activation : with
Result : negative
Method : other: modification of Schechtman and Kouri. In: Progress in Genetic Toxicology. D.Scott et al, eds. Elsevier/North Holland Biomedical Press, NY. pp.307-316.
Year : 1977
GLP : yes
Test substance : other TS: mixture of commercial DINPs
Remark : Test substance purity >98%.
01.06.2001 (3)

Type : other: cell transformation assay
System of testing : BALB/C 3T3 cells
Concentration : 0.01, 0.1, or 1.0 ul/ml
Cycotoxic conc. :
Metabolic activation : without
Result : negative
Method : other: modification of Schechtman and Kouri. In: Progress in Genetic Toxicology. D.Scott et al, eds. Elsevier/North Holland Biomedical Press, NY. pp.307-316.
Year : 1977
GLP : yes
Test substance : other TS: mixture of commercial DINPs
Remark : Test substance purity >98%.
01.06.2001 (2)

Type : other: cell transformation assay
System of testing : BALB/C 3T3 cells
Concentration : 0.03, 0.1, 0.3 or 1.0 ul/ml
Cycotoxic conc. :
Metabolic activation : without
Result : positive
Method : other: modification of Schechtman and Kouri. In: Progress in Genetic Toxicology. D.Scott et al, eds. Elsevier/North Holland Biomedical Press, NY. pp.307-316.
Year : 1977
GLP : yes
Test substance : other TS: mixture of commercial DINPs
Remark : Test substance purity >99.85%.
01.06.2001 (6)

Type : other: cell transformation assay

System of testing	:	BALB/C 3T3 cells
Concentration	:	2.5 to 254.5 ug/ml
Cycotoxic conc.	:	
Metabolic activation	:	without
Result	:	negative
Method	:	other: not specified
Year	:	
GLP	:	yes
Test substance	:	other TS: mixture of commercial DINPs

01.06.2001 (60)

5.6 GENETIC TOXICITY 'IN VITRO'

Type	:	Cytogenetic assay
Species	:	rat
Sex	:	male
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	5 consecutive days
Doses	:	0, 0.5, 1.7 or 5.0 ml/kg/day (approximately 500, 1700 and 5000 mg/kg/d)
Result	:	
Method	:	other: modification of Killian D.J. et al. In: Handbook of Mutagenicity Test Procedures. Kilbey B.J. et al, eds. Elsevier Scientific Publishing Company, NY. pp 243-260.
Year	:	1977
GLP	:	yes
Test substance	:	other TS: mixture of commercial DINPs
Remark	:	DINP did not increase the frequency of chromosomal aberrations in bone marrow cells and was not a mitotic inhibitor. In addition, no change in chromosome number was observed. Test substance purity >98%.

01.06.2001 (4)

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	CD-1
Route of admin.	:	gavage
Exposure period	:	one exposure
Doses	:	500, 1000, 2000
Result	:	negative
Method	:	other
Year	:	2000
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Schmid W. The micronucleus test. Mutat. Res. 1975; 31: 9-15. In vivo mammalian bone marrow micronucleus, oral gavage. Performed by Exxon Biomedical Sciences, Inc. (2000). Final Report.
Conclusion	:	DINP was inactive in an in vivo micronucleus test that utilized a multiple-treatment, single-sacrifice study design. Because an initial range-finding test had shown that there were no differences between males and females, the definitive test utilized male mice only. Frequency of micronucleus formation was not elevated at any dose and there was no evidence of toxicity.

01.06.2001 (102)

5.7 CARCINOGENITY

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	2 years
Frequency of treatment	:	daily
Post. obs. period	:	
Doses	:	0, 0.03, 0.3, and 0.6% (approximately 15, 150 and 300 mg/kg/d)
Result	:	
Control group	:	yes
Method	:	other: not specified
Year	:	1987
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Groups of 110 male and female Fisher 344 rats were given ad lib access to a diet containing DINP at dietary levels of 0, 0.03, 0.3, and 0.6% for periods up to 2 years. Interim sacrifices were done at 26, 52 and 78 weeks with surviving animals sacrificed at 24 months. At study termination, survivorship was in excess of 60% for all groups. At the MID and HIGH DOSES, the following biological effects were noted in both males and females: INCREASE IN RELATIVE ORGAN WEIGHTS (LIVER, KIDNEY); AND SOME MILD EFFECTS ON URINALYSIS/CLINICAL CHEMISTRY PARAMETERS. At the HIGH DOSE, a DECREASE IN BODY WEIGHT (4-7%), DECREASED FOOD CONSUMPTION, and MILD HEMATOLOGICAL CHANGES were seen in the males. Since the liver was identified as a potential target organ, a morphological exam of the liver was done. No evidence of peroxisome induction was observed in treated rats as compared to controls. Non-neoplastic and neoplastic lesions (i.e. liver tumors) of the anticipated type and incidence for this rat strain occurred in all groups. These lesions were not treatment related. There was a MARGINALLY INCREASED INCIDENCE OF MONONUCLEAR CELL LEUKEMIA (MNCL) IN THE HIGH DOSE GROUPS, however, the weight of evidence indicates that the effects of DINP on MCL are not biologically significant.
Conclusion	:	No liver tumors were observed. The NOEL for peroxisome induction was approximately 340 mg/kg/day.

26.04.2001 (25) (39) (99)

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	2 years
Frequency of treatment	:	daily
Post. obs. period	:	none
Doses	:	500, 1500, 6000, 12000 ppm (approximately 30, 100, 400 and 800 mg/kg/day).
Result	:	
Control group	:	yes
Method	:	EPA OPPTS 870.4200
Year	:	
GLP	:	yes

Test substance : other TS: DINP with same CAS# but produced by another manufacturer.
Remark : Groups of male and female Fischer 344 rats were fed DINP for 104 weeks, except for the recovery group animals (12000-R) which were given access to dietary DINP 78 weeks and then received untreated diet. At study termination, survivorship was in excess of 50% for all groups. An increased incidence of hepatocellular tumors (31%) was seen in the high dose males vs. controls (6%). However this effect appeared to be reversible based on the lower incidence observed in the recovery group (14%). High dose females had a 10% increase in hepatocellular tumors.
Conclusion : The no effect level for all effects was 1500 ppm (88 mg/kg/day for males and 109 mg/kg/day in females). The no effect level for tumor induction was 6000 ppm (approximately 400 mg/kg/day). Hepatocellular tumors were significantly elevated in both male and female rats by a peroxisomal proliferation process. As a consequence they are not clinically relevant to humans. Kidney tumors were elevated in the male rats in the high dose group and the control. These have been shown to be the consequence of an alpha 2u microglobulin-mediated process and without clinical relevance to humans.

01.06.2001 (14) (15) (32) (114)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : oral feed
Exposure period : 2 years
Frequency of treatment : daily
Post. obs. period : none
Doses : 500, 1500, 4000, 8000 ppm. (~ 100, 300, 800, 1600 mg/kg/day)
Result :
Control group : yes
Method : other: not specified
Year :
GLP : yes
Test substance : other TS: DINP with same CAS# but produced by another manufacturer.
Remark : Male and female B6C3F1 mice received 0, 5000, 1500 4000 or 8000 ppm di(isononyl)phthalate in their diets for up to 104 weeks. Extra animals received the 8000 ppm diet for 78 weeks followed by 26 weeks of control diet (recovery). Cell proliferation and peroxisome proliferation (PP) were determined after weeks 78 and 104. Survival was reduced in the 4000 and 8000 ppm groups for each sex in a dose-related fashion. Survival was better in the recovery groups but was still below control values. At week 105 male body weights were reduced 11.1% and 18.9% in the top two dose groups and 5.7% in the recovery group as compared to controls: female body weights were not reduced by more than 10% in any test grup and the recovery group showed a 5.7% reduction compared to controls. In male mice, incidences of hepatocellular carcinoma were increased above control levels in the 1500 ppm group (30% vs 23%), the 4000 ppm (47%), the 8000 ppm group (44%) and 38% in the recovery group. In female mice, the comparisons were 4% incidence in the controls, 17%, 18%, 46% and 36% in the 1500, 4000, 8000 and recovery groups, respectively. There were no test article-related increases in tumors of any other type reported. Non-neoplastic liver changes included increased pigment, cytoplasmic eosinophilia and hepatocellular enlargement in male and female mice in the high dose but not the recovery groups. Chronic progressive nephropathy was reported as a treatment-related effect in high dose female mice. Sections of testes with epididymides revealed no evidence of a DINP effect on spermatogenic activity. Biochemical analyses of high-dose and control liver tissue at weeks 78 and 104 revealed a statistically significant increase in liver weight, hepatocellular protein content, and palmitoyl CoA oxidase activity but not cellular labelling or DNA

content.

Conclusion : The overall no effect level for all effects was 500 ppm (90 mg/kg/day in males and 112 mg/kg/day in females). Liver tumors were significantly elevated at levels above 500 ppm in females and at levels above 1500 ppm (276 mg/kg/day) in males. No tumor type other than hepatocellular tumors was significantly elevated. The hepatocellular tumors were the consequence of a peroxisomal proliferation process in this species and not clinically relevant to humans.

26.04.2001 (13) (31) (41) (114)

5.8 TOXICITY TO REPRODUCTION

Type	:	Two generation study
Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	up to 26 weeks
Frequency of treatment	:	daily
Premating exposure period		
Male	:	ten weeks (6 weeks old)
Female	:	ten weeks (6 weeks old)
Duration of test	:	up to 26 weeks
Doses	:	0.2%, 0.4%, 0.8% (n=30/sex/group)
Control group	:	yes, concurrent no treatment
NOAEL Parental	:	.8 - %
NOAEL F1 Offspr.	:	.8 - %
NOAEL F2 Offspr.	:	.8 - %
Method	:	other: Directive 67/548/EEC, Part B and OECD Guideline 414
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The potential reproductive toxicity of di-isononyl phthalate was assessed in one and two-generation reproductive toxicity studies. Groups of 30 male and female CRL:CD(SD)BR rats were given DINP via dietary administration at levels of either 0.0, 0.5, 1, or 1.5% (one generation study) or 0.0, 0.2, 0.4, or 0.8% (two generation study). There were no changes in any of the classic reproductive parameters, i.e., mating, male or female fertility, fecundity, gestational index, or length of gestation in either study. The overall NOAELs for these effects were the highest dietary levels (%) tested ~ 500 mg/kg/day in the two generation study and 1000 mg/kg/day in the one-generation study. In the two-generation study there were no testicular effects in either the P1 males, exposed as juveniles and young adults or the P2(F1) offspring exposed in utero, through lactation, and continuously to terminal sacrifice. The NOAEL was 470 mg/kg/day. Offspring survival was reduced at the 1.5% level (~ 1100 mg/kg/day) but unaffected at the 1% level (~ 760 mg/kg/day). Offspring body weights were decreased both at postnatal day (PND 0) and during lactation; however, the PND 0 effects were only clearly related to treatment at the 1.5% level. Weights of offspring during lactation were significantly reduced but within the historical control range at dietary levels (%) below 1%. As there was rapid recovery at the lower levels, even though treatment continued, the toxicologic significance is unclear. Adult survival was unaffected at any level in either study, but weight gain was significantly reduced at the 1% level (~ 600 mg/kg/day). Liver and kidney weights were elevated at dietary level (%) above ~ 110 mg/kg/day, consistent with evidence from other studies of peroxisomal proliferation at these levels.
Conclusion	:	This study showed that DINP treatment did not affect fertility or male

reproductive development at doses of up to approximately 1000 mg/kg/day.

01.06.2001 (75) (149)

Type	:	other: Assessment of Male Reproductive Development
Species	:	rat
Sex	:	male
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	exposure of dams, gestational day 14 to postnatal day 4
Frequency of treatment	:	daily
Premating exposure period		
Male	:	
Female	:	
Duration of test	:	from conception to sexual maturity (approximately 90 days)
Doses	:	750 mg/kg/day
Control group	:	yes, concurrent vehicle
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Female SD rats were given DINP by oral gavage from GD14 to PND 3 at a single treatment level (750 mg/kg/day). The offspring were examined at various times until terminal sacrifice at times ranging from 3 to 7 months of age. The parameters which were examined included: (a) body weight and anogenital distance - unaffected by treatment. (b) Testicular examination on PND 3 - testes of treated male offspring were similar to control. (c) Inguinal examination of male pups - It was reported that one treated male had "suspected hemorrhagic testes" but this was not confirmed histologically. (d) Examination for aerolas on PND 13 - The incidence of areolas (22%) was reported as significantly different from control. (e) Examination for onset of puberty (preputial separation) - not affected by treatment. (f) Determine of serum testosterone at terminal sacrifice - not affected by treatment. (g) Examination for retained nipples, cleft phallus, vaginal pouch and hypospadias - Of 52 males examined, 2 had retained nipples (note that the presence of areolas at day 13 did not result in a significant incidence of retained nipples), none had cleft phallus, vaginal pouch or hypospadia. (h) Internal examination for undescended testes, atrophic testes, epididymal agenesis, prostatic and vesicular agenesis and abnormalities of the gubernacular cord - one of the male offspring was reported to have had bilateral testicular atrophy and another exhibited epididymal agenesis with hypospermia and fluid filled testes. None of the 52 male offspring examined had undescended testes, prostatic and vesicular agenesis or abnormalities of the gubernacular cord.
Conclusion	:	Treatment from GD14 to PND 4 with 750 mg/kg/day resulted in a statistically significant increase in areolas at day 13. However, when the animals reached sexual maturity, only 2 (of 52 males) had retained nipples. Other parameters were not different from control values.

23.04.2001 (79)

Type	:	other: Assessment of male reproductive development
Species	:	rat
Sex	:	male
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	21 days

Frequency of treatment	:	daily
Premating exposure period		
Male	:	
Female	:	
Duration of test	:	21 days
Doses	:	0.6, 1.2 and 2.5% (approx. 600, 1200 and 2200 mg/kg/day)
Control group	:	yes, concurrent no treatment
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	other TS: mixture of commercial DINPs
Remark	:	Juvenile male rats were given DINP in the diet at levels of 0.6, 1.2 and 2.5% for 3 weeks. At terminal sacrifice, the testes were weighed and then preserved in formalin for microscopic examination. The testes weights were unaffected, and there were no testicular lesions at any treatment level.
Conclusion	:	Administration of DINP to juvenile rats at levels up to 2.5% (approximately 2200 mg/kg/day) had no effect on testicular weight and did not produce histological changes in the testes.

01.06.2001 (23) (98)

Type	:	other: effects on male reproductive system
Species	:	rat
Sex	:	male
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	1 week
Frequency of treatment	:	daily
Premating exposure period		
Male	:	
Female	:	
Duration of test	:	1 week
Doses	:	0, 2%
Control group	:	yes
Method	:	other: not specified
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	No significant differences were observed between treated and control rats in the following: histopathology of the testes, degree of spermatogenesis, histopathology of the epididymis, liver, kidney, salivary gland, cervical lymph node, lung, eye, and gross lesion examination.

18.04.2001 (76)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	other: Crl:CDBR
Route of admin.	:	gavage
Exposure period	:	Gestation Days 6-15
Frequency of treatment	:	daily
Duration of test	:	21 days
Doses	:	0, 100, 500, and 1000 mg/kg/day

Control group	:	yes
NOAEL Maternalt.	:	= 500 - mg/kg bw
NOAEL Teratogen	:	= 500 - mg/kg bw
Method	:	Directive 87/302/EEC, part B, p. 24 "Teratogenicity test - rodent and non-rodent"
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	DINP was not a selective developmental toxicant, nor was it embryotoxic or teratogenic under conditions of this study.
Conclusion	:	The highest level (1000 mg/kg/day) reduced maternal weight gain and increased the incidence of developmental variations. The middose (500 mg/kg/day) was a NOAEL for both maternal and fetal effects.

18.04.2001 (148)

Species	:	rat
Sex	:	
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	Day 6 to 15
Frequency of treatment	:	Daily
Duration of test	:	Day 20
Doses	:	40, 200, 1000 mg/kg/day
Control group	:	yes
NOAEL Maternalt.	:	200 - mg/kg bw
NOAEL Teratogen	:	200 - mg/kg bw
Method	:	Directive 87/302/EEC, part B, p. 24 "Teratogenicity test - rodent and non-rodent"
Year	:	1987
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	A statistically significant increase in relative kidney weights noted in 1000 mg/kg/day dams. The only foetal effects were an increased occurrence of foetal skeletal variations consisting mainly of rudimentary cervical and/or accessory 14th rib(s) in the 1000 mg/kg/day group.
Reliability	:	(2) valid with restrictions

01.06.2001 (84)

5.10 OTHER RELEVANT INFORMATION

Type	:	other: Dermal Disposition
Remark	:	14C-labelled DINP was dermally applied to male F344 rats. A single dose of approximately 0.6 ml/kg or approximately 1.2 ml/kg was applied to the backs of the rats. An additional group of rats was pretreated with a dermal dose of nonlabeled DINP which was kept on the skin for 3 days, then blotted off prior to application of the 14C-labelled dose (approximately 1.2 ml/kg). The rates of absorption and excretion, as well as the levels of radioactivity in selected tissues were determined at 1, 3 or 7 days following treatment. Only 0.3% of the applied dose was recovered in the urine, feces and tissues at 24 hours. Dermal absorption of 14C-DINP was slow but occurred at a steady rate as evidenced by the increased amounts of radioactivity recovered in urine, feces and tissues examined at the later time periods. For all treatment conditions, the total amount absorbed at the end of the study ranged from 2 to 4% of the applied dose. Essentially all of the remaining doses

were recovered from the skin application areas.

07.06.2001 (43) (139)

Type : Toxicokinetics

Remark : The pharmacokinetic and metabolic behavior of [14C]-diisononyl phthalate (DINP) was investigated in male and female Fischer 344 rats treated with a single oral dose of 50 or 500 mg/kg, and in male rats treated with five daily oral doses of 50, 150 and 500 mg/kg. Elimination of radioactivity in urine and feces were examined for up to 72 hr after the last dose. Blood and tissue levels of radioactivity were determined in male rats sacrificed at 1, 4, 8, 24 and 72 hr and in females sacrificed at 24 hr. Liver tissues were subjected to subcellular fractionation and [14C] contents in selected tissues (liver, testes and fat) were examined by high performance liquid chromatography (HPLC).

In male rats receiving a single dose of [14C]-DINP, levels of radioactivity in blood and most tissues were highest at 1 hr following administration of both doses. The highest levels were demonstrated in liver (4.7 ± 0.07 % of administered dose ~ 53 mgEquiv./g), followed kidneys (0.31 ± 0.03% ~ 13m gEquiv./g), then blood (1.62 ± 0.07 %~ 11.6m gEquiv./g). At all times examined, most of the blood radioactivity was recovered in the plasma, in liver radioactivity was localized primarily in the cytosol. Radioactivity rapidly disappeared from blood, liver and kidney, reaching low levels at 72 hr (less than 0.05% of administered dose in the liver). Rates of disappearance from other tissues were slower. The levels in tissues were generally similar in the males and females treated at either dose levels.

In male and female rats, the entire administered radioactivity was essentially eliminated in urine (~ 49 % at low dose, ~ 39% at high dose) and feces (~ 51 % at either dose) within 72 hr after dosing; the major portions were eliminated within the first 24 hr. After the low dose, excretion in urine was initially higher than in feces, but by 72 hr, equal amounts were recovered in each. Following the high dose, elimination in urine and feces was initially equal (~ 38% at 24hr), but excretion in feces at 72 hr exceeded that in urine (~ 52% and ~ 39% respectively). In female rats, urinary and fecal excretion following the low or high doses was similar to that demonstrated for male rats.

Conclusion : The total amount of DINP recovered in the urine at 24 hours was about 93% of the total recovered in 96 hours. Assuming the total recovery at 96 hours to be approximately equivalent to the total absorbed, the elimination half time is approximately 6.3 hours.

01.06.2001 (54) (97) (107)

Type : Metabolism

Remark : Male albino rats received unlabelled DINP for 5 days. On the 6th day, they were dosed with 14C-DINP via oral intubation. Expired gases, fecal and urinary excreta were collected separately, at 12-hour intervals, for a period of 72 hours. Within 24 hours, over 90% of the recovered dose was excreted in the urine and feces. The major route of excretion was fecal by an 8 to 1 factor. No expired 14C-carbon dioxide was detected. Only 0.9% of the administered dose was retained after 72 hours.

18.04.2001 (105)

Type : other: Evidence of species differences in response based on in vitro studies (1)

Remark : Benford et al., 1986 investigated the peroxisome proliferation induction potential of DIDP monoester and DINP monoester (MiDP and MiNP respectively) and DINP in primary monolayer cultures of rat and marmoset monkey hepatocytes. Mono-(2-ethylhexyl) phthalate (MEHP) was used as a reference control. The measured parameters were peroxisomal

palmitoyl-CoA (PCoA) oxidation, laurate 11 - 12 hydroxylation (LAH) and the protein content of the homogenate.

In the rat hepatocytes culture, MiDP and MiNP were both peroxisome proliferators as indicated by marked dose-related increases in PCoA oxidation. The rank was in order MEHP >MiNP > DINP. DINP caused much smaller increases as it is poorly converted to the monoester in the culture system. LAH appeared to be more sensitive to induction by MiDP and MiNP than by MEHP, the rank was in order MiDP>MiNP>MEHP.

In the marmoset hepatocyte cultures, only minimal changes in PCoA oxidation activity were observed with MiDP, MiNP or DiNP with poor dose dependency and showed no changes with MEHP; MiDP and MiNP caused up to 4 and 3 fold increases in LAH activity (respectively). MEHP has no effect. A marked species difference has been observed in peroxisomal proliferation by phthalates in cultured hepatocytes.

26.04.2001 (21)

Type : adsorption

Remark : The ability of DINP to induce peroxisomal proliferation under in vitro conditions was investigated in rat and human hepatocytes. In the rat hepatocytes DINP induced peroxisomal enzymes and DNA synthesis and inhibited apoptosis. In human hepatocytes, DINP had no significant effects on any of these parameters. These data demonstrate species differences in responses to peroxisomal proliferating agents.

26.04.2001 (82)

Type : other: Evidence of species differences in response based on in vivo studies (1)

Remark : The objective of this study was to determine if DINP-induced effects in the liver are mediated by PPAR. Male and female SV129 PPAR-null (-/-), SV 129 PPAR (+/+) and B6C3F1 mice were fed a control diet or a diet containing 8000 ppm DINP for one week. There was an increase in relative liver weight in male and female PPAR (+/+) and B6C3F1 mice. The increase in liver weights was abolished in the 1 week treated male and female PPAR (-/-) mice. Western blot analysis of liver protein extracts demonstrated a strong induction of lipid metabolizing enzymes including acyl-CoA oxidase and Cyp4a proteins in PPAR (+/+) but not PPAR (-/-) male and female mice after DINP exposure. Preliminary experiments using DNA arrays containing 144 genes showed that 6 genes were altered in livers after a 3 week exposure in female PPAR (+/+) but not in PPAR (-/-) mice. These genes include those involved in drug metabolism and protein trafficking. These data support the hypothesis that DINP, like other PP induces liver effects through a PPAR-dependent mechanism.

20.04.2001 (147)

Type : other: Evidence of species differences in response based on in vivo studies (2)

Remark : The short term hepatic effects of DINP in rats and mice at tumorigenic and non-tumorigenic doses were evaluated for comparison with chronic studies and with data for other structurally similar dialkyl phthalate esters ranging from C7 to C11.

When given to rats at 12000 ppm in the diet, a tumorigenic dose, evidence of peroxisomal proliferation including liver weight increases, elevated liver enzyme levels, and elevated DNA synthesis were observed. Gap junctional intercellular communication (GJIC) was inhibited. None of these effects was altered when the rats were given 1000 ppm, a non-tumorigenic dose.

When given to mice at 6000 ppm in the diet, a tumorigenic dose, evidence of peroxisomal proliferation including liver weight increases, elevated liver enzyme levels and elevated DNA synthesis were observed.

GJIC was inhibited. These parameters were not affected at 500 ppm in this study.

These data provide evidence that DINP induces peroxisomal proliferation under the conditions of the bioassays in rats and mice.

01.06.2001 (132)

Type : other: Inhibition of Gap Junctional Intercellular Communication - in vivo

Remark : The effects of several phthalate esters including DINP on gap junctional intercellular communication were investigated under in vivo conditions. Hepatic GJIC was inhibited in B6C3F1 mice at DINP levels of 6000 ppm but not at 500 ppm. Hepatic GJIC was inhibited in Fischer 344 rats at 12,000 ppm but not at 1000 ppm.

In the cynomolgus monkey, hepatic GJIC was not inhibited by 500 mg/kg bw/day DINP administered by oral gavage on a daily basis for two weeks.

26.04.2001 (124) (132)

23.04.2001

Type : other: Inhibition of Gap Junctional Intercellular Communication - in vitro

Remark : Baker et al., 1996 examined GJIC (Gap Junctional Intercellular Communication) effects in hepatocytes of 4 species (rats, mice, hamsters, humans) for 5 phthalate monoesters (MINP-M, MINP-S, MEHP< MNOP< M711P) which are metabolites of the following diesters: two types of diisononyl phthalate (DINP-1 and DINP-A)di-2-ethy hexyl phthalate, di-n-octyl phthalate and diheptyl undecyl phthalate respectively.

In rat hepatocytes, all 5 monoesters inhibited GJIC. In mouse hepatocytes MEHP, M711P and MINP-S inhibit GIJC but not MINP-M and MNOP. In hamster or human hepatocytes and in a human liver cell line, none of the 5 monoesters inhibited GIJC at non-cytoxic doses. According to the authors, GJIC assay has good cancer predictive potential for phthalates.

23.04.2001 (18)

Type : other: Kidney Cancer Mechanistic Study (1)

Remark : A recent study conducted at dietary levels up to 1.2% DINP (~ 733 mg/kg/day for male rats) reported kidney tumors in male rats at the high treatment level but not in female rats or mice of either sex. Because these tumors occurred only in male rats, and only at high doses, the male rat-specific alpha 2u-globulin (a2UG) mechanism of action was investigated. Technological advances in immunohistochemical staining and computerized image analysis techniques permitted measurement of the accumulation of a2UG in archived kidneys from an earlier study (Lington et al., 1997). Using archived tissue obtained from the 12 month interim sacrifice, a dose dependent accumulation on a2UG was identified in specific regions of male rat kidneys only. An increase in cell proliferation was confirmed by immunohistochemical detection of proliferating-cell nuclear antigen (PNCA) and was confined to the areas of a2UG accumulation. H and E-stained sections revealed tubular epithelial hypertrophy and regeneration, consistent with the immunohistopathology findings. These findings are consistent with the a2UG mechanism of tumorigenesis which is not considered relevant to humans. In summary, exposure to DINP produced a dose-dependent accumulation of a2UG in male rat kidneys which was significant at a dietary level of 0.6% and a likely mechanism for the kidney tumors seen only in male rats given higher dietary levels of DINP.

26.04.2001 (35)

Type : other: Kidney Cancer Mechanistic Study (2)

Remark : Data summarized above suggest that DINP induces male rat specific a2U - globulin (a2UG) nephropathy. A series of studies was conducted to further investigate this issue. In the first study, reversible binding between DINP

and a2UG was evaluated. Male and female Fischer 344 (F344) rats were gavaged with a single dose (900 mg/kg) of radiolabeled [14C] - DINP. Kidney cytosol samples were pooled by gender, and dialyzed against buffer with or without 0.1 % SDS. Cytosol dialyzed against buffer with SDS, but not without SDS, lost radioactivity to background levels, demonstrating reversible binding of DINP to a2UG. A second study was done using immunohistochemistry (IHC) to quantify dose dependent accumulation of a2UG and changes in cell proliferation in kidneys of rats exposed to DINP. Male F344 rats were gavaged (90, 300 or 900 mg/kg) daily for 5 days. A negative and positive control group received corn oil or d-limonene, respectively. Animals received BrdU in drinking water for 72 hours prior to sacrifice. IHC showed an increase in the amount of a2UG staining in the treated over control groups. BrdU cell proliferation was measured to establish a labeling index (LI). When random fields of 2,000 cells were counted, large standard errors (SE³0.5) were present. This was due to localized lesions within the cortex which were counted or missed due to selection. Using counts of 10,000 and 20,000 cells, most of the cells cortex were counted with a SE<0.2 in all groups. There was a doubling in cell proliferation of DINP treated over control groups. Collectively, these data demonstrate that DINP induces a2UG nephropathy.

01.06.2001 (128)

Type : other: Mononuclear Cell Leukemia (MNCL)
Remark : A clear increase in MNCL incidence was observed in the two studies conducted with Fisher rats, along with shortening of the onset of MNCL. However, MNCL is a common neoplasm in the Fischer 344 rats with a high and variable incidence. The increased incidence after chronic exposure to some substances is likely a strain specific effect with little relevance for humans. Of interest, the IARC categorized MNCL as "an unclassified leukemia with no known human counterpart" and substances which increase MNCL frequency as "not classifiable as to carcinogenicity in humans." (IARC, 1990).

26.04.2001 (34)

Type : other: Endocrine Modulator (1)
Remark : DINP was tested in vitro for (a) Estrogen Receptor (ER) competitive ligand binding, and (b) gene expression in Mammalian and yeast-based gene expression assays. DINP was inactive in all of these in vitro assays.

DINP was also tested for estrogenic activity in vivo using the Uterotrophic assay/ vaginal cell cornification assay : 20, 200, 2,000 mg/kg/d of DINP were administered by oral gavage once daily for a period of 4 days to ovariectomized Sprague-Dawley rats (10 females per dose, two experiments). Ethynyl Estradiol (EE) was used as a positive control. Body weight, uterine wet weight and percentage of vaginal epithelial cell cornification on each day were assessed.

Neither DINP nor any of the other phthalate esters tested had a reproducible, dose-dependant effect on uterine wet weight relative to vehicle control at any of the doses tested. Additionally, none of the phthalate esters tested induced a significant vaginal cornification response at any of the doses tested.

26.04.2001 (153)

Type : other: Estrogenic Activity (2)
Remark : Di-isononyl phthalate was inactive in a competitive binding assay for the estrogen receptor.
DINP, and a number of other commercially available phthalates were screened for estrogenic activity in a recombinant yeast assay. DINP behaved unreproducibly in the screen, displaying estrogenic activity in some assays and no

acitivity in others. The relative potencies, based on the yeast assay, was determined to be: butybenzyl phthalate > dibutyl phthalate > diisobutyl phthalate > diethyl phthalate > diisononyl phthalate. Potencies in this assay ranged from approximately one million to 50 million times less than 17 B-estradiol. These phthalates were also found to be mitogenic to breast cancer cells in vitro. Attention was drawn to the observation that some of the phthalate diesters were active in these in vitro screening tests but that the monoesters, the forms encountered under in vivo conditions, are inactive.

Reliability : (4) not assignable
23.04.2001 (81)

Type : other: Estrogenic Activity (3)
Remark : Di-nonyl phthalate did not compete with estrogen for binding to the estrogen receptor. The ER was obtained from rainbow trout.
23.04.2001 (94)

Type : other: Estrogenic Activity (4)
Remark : DINP did not compete for the estrogen receptor.
23.04.2001 (27)

5.11 EXPERIENCE WITH HUMAN EXPOSURE

Memo : Sources of General Exposure (Air)
Remark : The levels of DINP in air have been quantified in two publications. The first (Wechsler, 1984) collected aerosol in indoor and outdoor locations. The levels of DINP in indoor air at two locations in the US were reported as 15 ng/m3. DINP was not detectable in outdoor air. The second study (Tienpont et al., 2000) using a thermal desorption method, reported that levels of DINP in air from both indoor and outdoor sources were below quantitation limits (20 ng/m3). Data from Oie et al., (1997), showing that DINP is below detection limits in indoor suspended dust provide additional evidence that the DINP levels in air were not underestimated in the other studies.
20.04.2001 (113) (145) (150)

Memo : Sources of General Exposure (Dust)
Remark : Oie et al., (1997) reported dinonyl phthalate in dust at levels of 10 ug/100 mg sedimented dust, equivalent to 100 mg/kg. Dinonyl phthalate was not found in suspended dust. In a subsequent study, (Pfordt and Bruns-Weller), dinonyl phthalate levels in dust were reported to range from below detection (10 mg/kg) to 20 mg/kg.
01.06.2001 (112) (119)

Memo : Sources of General Exposure (Food)
Remark : MAFF's Food safety directorate has carried out a survey of the levels of total and individual phthalates in samples of composite fatty foods from the Total Diet Study (TDS). The survey was carried out using stored samples of food that had been collected in 1993.

Di-isononyl phthalate levels were reported as below detection limits in both food (MAFF 1996a) and baby food (MAFF 1996b; 1998).

In a second study (Pfordt and Bruns-Weller, 1999), DINP levels were below the limits of detection (10 ppb) in milk, cream, baby food, and breast milk. Levels ranging from 10-60 ppb were found in nuts.
20.04.2001 (100) (120)

19.04.2001

Memo : Urinary Metabolite Data
Remark : Using a novel and highly selective technique, monoester metabolites of seven commonly used phthalates were measured in urine samples from a reference population of 289 adult humans (Blount et al., 2000). This analytical approach allowed direct measurements of the individual phthalate metabolites while avoiding contamination from the ubiquitous parent compounds. The reported levels in ng/ml were...

Phthalate	50th percentile	95th percentile	Geometic mean
isononyl	< LOD	7.3	1.5

when normalized for urinary creatinine, the values become

isononyl	< LOD	6.8	1.3

These values were then used to external exposure by two different groups. The estimates, which differ slightly are, in ug/kg/day...

Phthalate	geometic mean	95th percentile	Reference
DINP	0.21	1.08	David, 2000
DINP	*	1.7	Kohn, 2000

A subsequent study (CDC, 2001)involving approximately 1000 individuals, representing a cross section of the US population, found similar data. The reported urinary levels in ng/ml were...

phthalate	50th percentile	90th percentile	geometic mean
isononyl	< LoD	4.3	*

* not calculated because the proportion of results below the limit of detection was too high to provide a valid result.

26.04.2001 (28) (42) (95) (110)

19.04.2001

Memo : other: Exposure to DINP via the water
Remark : DINP has seldom been detected in either surface water or drinking water (see section 3.2). However, as a worst case assessment, a concentration equivalent to the water solubility limit can be used in exposure calculations. Careful experimental measurements and theoretical predictions reported in section 2.6 indicate that the water solubility of DINP is < 1 ug/L. Assuming 2 liters of water are consumed per day, this yields a maximum exposure of 0.03 ug/kg/day for a 70 kg person.
Water 5.11.2.2

26.04.2001

19.04.2001

Memo : Other: Exposures during manufacture and use of DINP
Remark : Monitoring data collected over several years to assess occupational exposure of process operations and maintenance technicians at a plasticizer plant indicate DINP concentrations in air of <2 mg/m3. Assuming 10m3 of air is inhaled per working day, 220 working days per year, and 40 working years over a 70 year lifetime, the estimated occupational exposure for a 70 Kg individual is <100 ug/kg/day.
A recent monitoring study was performed at a Volkswagen processing plant in Germany that uses DINP and DEHP in product applications. DINP measurements were made in several locations that were expected to yield the highest

workplace exposure concentrations. Results indicated DINP concentrations ranged from < 0.001 to 0.029 mg/m3. Similar concentrations were obtained for DEHP. Using the highest air concentration measured, a maximum DINP exposure of 1 ug/kg/day is obtained using the assumptions stated previously.
Occupational Exposure 5.11.1

23.04.2001 (74)

Memo : other: Exposures during DINP manufacture
Remark : Industrial hygiene surveys during 1983, 1986, 1988 and 1994 have been conducted at a plasticizer plant in the United States. Monitoring data indicate that DINP concentrations are usually not observed above an analytical detection limit of approximately 0.05 mg/m3. This translates into a maximum exposure of 2.5 ug/kg/day using the assumptions stated previously. Results from these studies should be directly applicable to Europe since production facilities are operated similarly.

26.04.2001 (86) (89) (90) (91) (92)

19.04.2001

Memo : other: estimates of phthalate exposure (1)
Remark : Independent estimates of the total daily intake of DEHP reported by various investigators are summarized below:

1 - 4 ug/kg/day CEFIC (1985)
5.8 ug/kg/day Canada (1993)
4 ug/kg/day ASTDR (1993)
0.1 - 0.5 ug/kg/day ECETOC (1994)

Limited data are availiable to estimate the total daily intake of DINP through multiple exposure routes. However, exposures to DINP are unlikely to exceed those estimated for DEHP and may be substantially lower.
Multiple Exposure Routes 5.11.2.4

20.04.2001 (12) (37) (38) (46)

20.04.2001

Memo : other: estimates of phthalate exposure (2)
Remark : In a recent study by Dutch Authorities, the total daily intake of "total" phthalates was estimated to be 7.3 ug/kg/day with an upperbound estimate of 21 ug/kg/day. If these estimates are weighted by relative production volume of the various phthalates, to "total" phthalates, these estimates of exposure to DEHP and DINP agree closely with exposure estimates provided above.

20.04.2001 (118)

Memo : other: exposure to DINP via food
23.04.2001

20.04.2001

(1) 13 Week Dietary Administration - Dogs. Report prepared by Hazleton Laboratories, Inc. and submitted to Esso Research and Engineering Co. Report date January, 1971.

(2) Activity of T1646 in the In Vitro Mammalian Cell Transformation Assay in the Absence of Exogenous Metabolic Activation. Performed by Microbiological Associates for Tenneco Chemicals, Inc. (1981). Final report. EPA Document No. 878210232.

(3) Activity of T1646 in the In Vitro Mammalian Cell Transformation Assay in the Presence of Exogenous Metabolic Activation. Performed by Microbiological Associates for Tenneco Chemicals, Inc. (1981). Final Report. EPA Document No. 878210236.

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7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 68515-49-1
CAS No.	:	68515-49-1
EINECS Name	:	1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
EINECS No.	:	271-091-4
Molecular Weight	:	446
Structural Formula	:	c(ccc1C(=O)OCCC(C)CCC(C)CC)cc1C(=O)OCCC(C)CCC(C)CC
Molecular Formula	:	C2804H46

Producer Related Part

Company	:	Exxon Chemical Holland BV
Creation date	:	21.12.1992

Substance Related Part

Company	:	Exxon Chemical Holland BV
Creation date	:	21.12.1992
Memo	:	
Printing date	:	13.11.2001
Revision date	:	21.12.1992
Date of last Update	:	10.09.2001
Number of Pages	:	56
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

Substance type : organic
Physical status : liquid
Purity : > 99.7 - % w/w
Remark : C9-C11 branched dialkyl ester, C10 rich.
Smiles code for typical isomers.

13.02.1996

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

DIDP
13.02.1996

Diisodecyl Phthalate
22.12.1992

Jayflex DIDP
Remark : In the "oxo industry", the term "iso" denotes a mixture of isomers and does not refer to the IUPAC definition.

13.02.1996

1.3 IMPURITIES

CAS-No :
EINECS-No :
EINECS-Name : Isodecyl ether
Contents : - % w/w
13.02.1996

CAS-No :
EINECS-No :
EINECS-Name : Isodecyl benzoate
Contents : - % w/w
13.02.1996

CAS-No :
EINECS-No :
EINECS-Name : Water

Contents : - % w/w
Remark : Diisodecyl ether and Isodecyl benzoate content ca. 0.07% w/w
The above average mentioned impurities have been identified.
13.02.1996

CAS-No : 93821-11-5
EINECS-No :
EINECS-Name : Isodecyl alcohol
Contents : ca. .05 - % w/w
13.02.1996

1.4 ADDITIVES

CAS-No : 80-05-7
EINECS-No :
EINECS-Name : Phenol, 4,4'-(1-methylethylidene)bis
Contents : .5 - % w/w
Remark : Added only when specifically requested by customer.
30.01.1996

1.5 QUANTITY

Remark : Please refer to proprietary document for description of quantities produced.
20.03.1996

1.6.1 LABELLING

Labelling : no labelling required (no dangerous properties)
07.04.1995

1.6.2 CLASSIFICATION

Classification : no classification required (no dangerous properties)
Class of danger :
R-Phrases :
07.04.1995

1.7 USE PATTERN

Type : type
Category : Use resulting in inclusion into or onto matrix
30.01.1996

Type : industrial
Category : Polymers industry
30.01.1996

Type : industrial
Category : other: plasticizer
02.02.1996

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit : MAC (NL)
Limit value : 5 mg/m3
13.02.1996

Type of limit : OES (UK)
Limit value : 5 mg/m3
30.01.1996

Type of limit : TLV (US)
Limit value : 5 mg/m3
Short term exposure
Limit value : 10 mg/m3
Schedule : 15 minute(s)
Frequency : 1 times
Remark : Data for Di-2-ethylhexyl Phthalate
13.02.1996

Type of limit : other
Limit value : 5 mg/m3
Remark : Exxon recommended Occupational Exposure Limit
13.02.1996 (47)

Type of limit : other: MAK (Germany)
Limit value : 10 mg/m3
Remark : Data for Di-2-ethylhexyl Phthalate
13.02.1996

Type of limit : other: OEL (Finland)
Limit value : 5 mg/m3
Remark : Data for Di-2-Ethyl hexyl phthalate
30.01.1996

Type of limit : other: OEL (Norway)
Limit value : 3 mg/m3
Remark : Data for Di-2-Ethyl hexyl phthalate
30.01.1996

Type of limit : other: OEL (sweden)
Limit value : 3 mg/m3
30.01.1996

Type of limit : other: TLV (DE)
Limit value : 3 mg/m3
Remark : Data for Di-2-ethylhexyl Phthalate
13.02.1996

Type of limit : other: VME (France)
Limit value : 5 mg/m3
Remark : Data for Di-2-Ethyl hexyl phthalate
30.01.1996

1.9 SOURCE OF EXPOSURE

Remark : The manufacturing process for DIDP is within a closed system under vacuum. The different sources of exposure during manufacturing, distribution, processing, use and disposal are described in detail by Cadogan, et al. (1994). Further information on the use of plasticizers and general equipment and process descriptions can be found in the additional references cited below:

20.03.1996 (23) (49) (76) (94) (103) (109) (120) (126)

1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES

1.10.2 EMERGENCY MEASURES

1.11 PACKAGING

1.12 POSSIB. OF RENDERING SUBST. HARMLESS

1.13 STATEMENTS CONCERNING WASTE

1.14.1 WATER POLLUTION

1.14.2 MAJOR ACCIDENT HAZARDS

1.14.3 AIR POLLUTION

1.15 ADDITIONAL REMARKS

Remark : See Safety Data Sheet
30.01.1996

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value	:	ca. -50 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	other: ASTM D97
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Pour Point

30.01.1996 (46)

2.2 BOILING POINT

Value	:	> 250 - ° C at 1013 hPa
Decomposition	:	no
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	

13.02.1996 (112)

2.3 DENSITY

Type	:	relative density
Value	:	= .971 - g/cm3 at 15° C
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	

25.04.1995 (62)

Type	:	density
Value	:	= .966 - g/cm3 at 20° C
Method	:	other: ASTM D4052
Year	:	
GLP	:	no data
Test substance	:	

03.01.1996 (46)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	.0000000000031 - hPa at 25° C
Decomposition	:	
Method		other (calculated): no further information
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Calculated using U.S. Environmental Protection Agency's Quantitative Structure Activity Relationship Program.

16.10.1995 (106)

Value : = .0000000184 - hPa at 25° C
Decomposition :
Method
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : QSPR estimate.
Source : ExxonMobil Biomedical Sciences, Inc.
05.06.2001 (33)

Value : < .00000072 - hPa at 25° C
Decomposition :
Method other (measured): Gas Saturation
Year :
GLP : yes
Test substance :
Remark : Value based on experimental results for di-iso-nonyl phthalate and the observed inverse relationship between the vapor pressure and alkyl chain length reported in this study.
13.02.1996 (57)

Value : ca. .5 - hPa at 200° C
Decomposition :
Method other (measured)
Year :
GLP :
Test substance :
Remark : Extrapolation to 25C yields an estimate of 0.00000008 hPa
13.02.1996 (110)

2.5 PARTITION COEFFICIENT

Log pow : > 8.6 - at 25° C
Method other (measured): HPLC retention time
Year : 1985
GLP : yes
Test substance :
Remark : More precise estimates cannot be determined since retention of DIDP exceeded that of the highest standard.
21.03.1996 (58)

Log pow : 9.3 - at ° C
Method other (measured): HPLC retention time
Year : 1995
GLP : no data
Test substance :
20.03.1996 (107)

Log pow : = 9.46 - at 25° C
Method
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : QSPR estimate
Source : ExxonMobil Biomedical Sciences, Inc.
05.06.2001 (33)

Log pow : 10.8 - at 25° C

Method other (calculated): U.S. Environmental Protection Agency's Quantitative Structure Activity Relationship Program
Year : 1991
GLP : no data
Test substance :
13.10.1995 (106)

2.6.1 WATER SOLUBILITY

Value : < .00013 - mg/l at 21 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other: "Slow-Stir" Shake Flask
Year :
GLP : yes
Test substance :
Remark : The procedure for this study involved adding TS to several glass vessels containing 4 liters of carbon-treated well water to yield a nominal concentration of 100 mg/l. Each glass vessel contained a glass stir bar and was gently stirred with the aid of a stir plate. The TS which existed as a visible surface film of free product was allowed to equilibrate with the water in which it was in contact for a period of up to 9 days. After 3 and 9 days of equilibration, a 3 liter sample was removed from a port at the bottom of the vessel (thus minimizing sample contamination from free product on the surface) for DIDP analysis. Three test vessels were sampled in this manner at each time period in order to provide triplicate analyses for water solubility determination. Analyses first involved passing the aqueous sample through a solid phase extraction cartridge, eluting the cartridge with solvent, followed by subsequent concentration of the extract by solvent evaporation. This extract was then analyzed using GC/MS in the selective ion monitoring (SIM) mode. Special precautions were taken in this study to minimize laboratory contamination. Recoveries for samples spiked at 0.0006 mg/l were 97% using this procedure. Measured water solubilities for DIDP were below analytical detection limits that ranged from < 0.00003 to < 0.00013 mg/l.
21.03.1996 (42)

Value : 0 - .00005 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other: (calculated) based on measured Log Kow
Year :
GLP : no data
Test substance :
13.02.1996 (108)

Value : 0 - mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other: (calculated) - U.S. Environmental Protection Agency's Quantitative Structure Activity Relationship Program
Year :

GLP :
Test substance :
13.02.1996 (106)

Value : = .00004 - mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : QSPR estimate.
Source : ExxonMobil Biomedical Sciences, Inc.
05.06.2001 (33)

Value : 1.19 - mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other: (measured) conventional shake flask
Year :
GLP :
Test substance :
Remark : Due to experimental difficulties associated with this method when applied to poorly water soluble materials the results of this study are believed to significantly overestimate the true water solubility by several orders of magnitude.
13.02.1996 (58)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : > 200 ° C
Type : closed cup
Method : other: (ASTM D93)
Year :
GLP : no data
Test substance :
30.01.1996 (46)

Value : 212 ° C
Type : closed cup
Method : other: Pensky-Marten closed cup
Year :
GLP : no data
Test substance :
25.04.1995 (62)

2.8 AUTO FLAMMABILITY

Value : > 260 - ° C at 1013.25 hPa
Method : other: not specified
Year :
GLP : no data
Test substance :

Remark : Value refers to autoignition temperature.
30.01.1996 (46)

2.9 FLAMMABILITY

Result : other: unclassified
Method : other
Year :
GLP : no data
Test substance :
Remark : Flash point higher than 100 degree C.
21.03.1996 (30)

2.10 EXPLOSIVE PROPERTIES

Result : no data
Remark : The lower explosive limit for Di-2-ethylhexyl phthalate is 0.28% in air at 246 degrees C.
18.03.1996 (111)

2.11 OXIDIZING PROPERTIES

Result : other: not applicable
Remark : Phthalate esters have no known oxidizing properties.
30.01.1996

2.12 ADDITIONAL REMARKS

Remark : Surface Tension

Value: 30-34 mPa.M

Method: not specified
13.02.1996 (111)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	- based on Intensity of Sunlight
Indirect photolysis		
Sensitizer	:	other: OH radical
Conc. of sens.	:	.00003 molecule/cm3
Rate constant	:	.000000000026 cm3/(molecule*sec)
Degradation	:	50 - % after 2.1 day
Deg. Product	:	
Method	:	other (calculated): Atmospheric Oxidation Program
Year	:	1993
GLP	:	no data
Test substance	:	
Remark	:	Estimated half-life of 2.1 days.

03.11.1995 (89)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

Type of measurement	:	background concentration
Medium	:	sediment
Method	:	
Concentration	:	-
Remark	:	Sediments from 8 lakes in Sweden and 10 sample locations in a Swedish river system which provided a gradient of anthropogenic influence were analyzed for DIDP in 1994. A total of 54 sediment analyses were performed on samples collected from these locations. DIDP was not detected in any sample (Estimated detection limit of <0.02 mg/kg dry wt).

21.03.1996 (100)

Type of measurement	:	background concentration
Medium	:	food
Method	:	
Concentration	:	-
Remark	:	Food samples of jam, pickels and sauces from containers with closure seals containing 25-40% DIDP were analyzed during the late 1980's. DIDP was not detected in any sample at a detection limit of 1 mg/kg (N=10).

13.02.1996 (92)

Type of measurement	:	concentration at contaminated site
Medium	:	sediment
Method	:	
Concentration	:	-
Remark	:	Sediments were collected downstream of two point source discharges. Mean DIDP concentrations above and below both

point sources were below detection limits <0.02 mg/kg dry wt, in all three samples collected at each station. Sediment concentrations at stations upstream of both point sources were below detection limits.

18.03.1996 (101)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : other: sediment - water
Method : other (measurement): U.S. Environmental Protection Agency Protocol for determining sediment and soil adsorption isotherms
Year : 1995
Remark : Experimental Koc values were defined as the ratio of chemical concentration in sediment organic carbon to the concentration in water (free + colloid-bound). The value below is the mean obtained from experiments with three different sediments. Experimental data were also corrected for "particle-effects" yielding a mean particle-corrected Koc value of 39,800,000 l/kg sediment organic carbon.
Result : 2,860,000 l/kg sediment organic carbon

18.03.1996 (127)

3.4 MODE OF DEGRADATION IN ACTUAL USE

Remark : If extracted from the matrix into which DIDP is included, biodegradation and photodegradation are believed to be the main modes of degradation.

04.06.2001 (22)

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge
Concentration : 100mg/l related to Test substance
related to
Contact time :
Degradation : 39 - % after 28 day
Result :
Deg. Product :
Method : OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year : 1990
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

18.03.1996 (77)

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 100mg/l related to Test substance
related to
Contact time :
Degradation : 54 - % after 28 day
Result :

Kinetic of test substance : 5 day 2 - %
10 day 28 - %
15 day 43 - %
20 day 49 - %
- %

Deg. Product :
Method : OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year : 1984
GLP : no
Test substance : other TS: Di-isodecyl phthalate (DIDP) mixed with a small quantity of the equivalent 14C carbonyl group radiolabelled substance in acetone solution. The acetone was removed by evaporation.

18.03.1996 (64)

Type : aerobic
Inoculum : other: activated sludge, unacclimated
Concentration : 100mg/l related to
related to
Contact time :
Degradation : 67 - % after 28 day
Result : readily biodegradable
Deg. Product :
Method : OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year :
GLP : no data
Test substance : no data

02.02.1996 (118)

Type : aerobic
Inoculum : other: activated sludge, unacclimated
Concentration : 35mg/l related to Test substance
related to
Contact time :
Degradation : 67.1 - % after 28 day
Result : readily biodegradable
Kinetic of test substance : 7 day = 0 - %
14 day = 27.7 - %
21 day = 56 - %
- %
- %

Deg. Product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

02.02.1996 (40)

Type : aerobic
Inoculum : activated sludge
Concentration : 100mg/l related to Test substance
related to
Contact time :
Degradation : 42 - % after 14 day
Result :
Deg. Product :
Method : OECD Guide-line 302 C "Inherent Biodegradability: Modified MITI Test (II)"
Year :
GLP : yes
Test substance : other TS: CAS # different

Remark : Upward trend noted at end of experiment suggesting initial lag phase.

18.03.1996 (29)

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 3mg/l related to Test substance related to
Contact time :
Degradation : >= 90 - % after 9 day
Result : inherently biodegradable
Deg. Product :
Method : other: Die-Away Test
Year :
GLP : yes
Test substance : other TS: CAS # different
Remark : Results are categorized as "inherently" rather than "readily" biodegradable since an adapted inoculum was used.

21.03.1996 (32) (96)

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 1mg/l related to Test substance related to
Contact time :
Degradation : 68 - % after 24 hour(s)
Result : inherently biodegradable
Deg. Product :
Method : other: Semi-Continuous Activated Sludge (SCAS)
Year :
GLP : yes
Test substance : other TS: CAS # different
Remark : Results are categorized as "inherently" rather than "readily" biodegradable since an adapted inoculum was used.

21.03.1996 (32) (96)

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 20mg/l related to Test substance related to
Contact time :
Degradation : 56 - % after 28 day
Result : inherently biodegradable
Kinetic of test substance : 3 day = 1 - %

7 day = 5 - %
9 day = 17 - %
14 day = 39 - %
21 day = 53 - %

Deg. Product :
Method : other: Shake Flask Test - CO2 Evolution
Year :
GLP : yes
Test substance : other TS: mixture of different commercial DINP products
Remark : Primary degradation based on disappearance of parent compound was > 99% after 28 days.
Results are categorized as "inherently" rather than "readily" biodegradable since an adapted inoculum was used.

20.03.1996 (117)

Type : aerobic
Inoculum : activated sludge

Concentration	:	100mg/l related to Test substance related to
Contact time	:	
Degradation	:	75 - % after 28 day
Result	:	
Deg. Product	:	
Method	:	other: modified OECD 301C to include determination of biodegradability by measuring DOC (Dissolved Organic Carbon) removal.
Year	:	1990
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

04.06.2001 (77)

Type	:	aerobic
Inoculum	:	activated sludge, adapted
Concentration	:	100mg/l related to Test substance related to
Contact time	:	
Degradation	:	88 - % after 28
Result	:	inherently biodegradable
Deg. Product	:	
Method	:	other: the OECD Guideline 301C was amended to include a determination of biodegradability by measuring carbon dioxide 14CO2 evolution.
Year	:	1984
GLP	:	no
Test substance	:	other TS: Di-isodecyl Phthalate mixed with a small quantity of the equivalent 14C carbonyl group radiolabelled substance in acetone solution. The acetone was removed by evaporation.

18.03.1996 (65)

3.6 BOD5, COD OR BOD5/COD RATIO

COD		
Method	:	
Year	:	1984
GLP	:	
COD	:	mg/g substance

23.12.1992

3.7 BIOACCUMULATION

Species	:	Cyprinus carpio (Fish, fresh water)
Exposure period	:	56 day at degree C
Concentration	:	1mg/l
BCF	:	< 3.6 -
Elimination	:	no
Method	:	OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"
Year	:	
GLP	:	yes
Test substance	:	other TS: different CAS #
Remark	:	Fish weight about 30 grams; lipid content 2-6%.

18.03.1996 (29)

Species	:	Cyprinus carpio (Fish, fresh water)
Exposure period	:	56 day at degree C
Concentration	:	.1mg/l
BCF	:	< 14.4 -

Elimination : no
Method : OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"
Year :
GLP : yes
Test substance : other TS: different CAS #
Remark : Fish weight about 30 grams; lipid content 2-6%.
18.03.1996 (29)

Species : other: Daphnia magna
Exposure period : 21 day at 20 degree C
Concentration :
BCF : 116 -
Elimination :
Method : other: not reported
Year :
GLP : no data
Test substance : other TS: 14C radiolabeled DIDP in acetone; chemical and radiochemical purity was 98%
Remark : BCF based on mean of reported values ranging from 90 to 147.
BCF is based on total radioactivity (parent compound and metabolites) and may significantly overestimate the extent to which DIDP is bioconcentrated.
Nominal Concentration.
3.2 to 100 ug/L.
21.03.1996 (14)

Species : other: Chiromonus riparius
Exposure period : 28 day at degree C
Concentration :
BCF : .6 -
Elimination :
Method :
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : BCF based on total radioactivity (parent compound and metabolites) and may significantly overestimate the extent to which parent DIDP is bioconcentrated.
BCF expressed as concentration in animals on a dry weight basis at end of 28 day sediment exposure divided by concentration in the sediment on a dry weight basis.
Chiromonids were exposed to river sediments spiked with DIDP at concentrations of 100, 1000 and 10,000 mg/kg/day. Tissue concentrations were analyzed at the end of the 28 day sediment exposure.
04.06.2001 (20)

Species : other: Mytilus edulis
Exposure period : 28 day at 15 degree C
Concentration :
BCF : 3500 -
Elimination : yes
Method : other: not specified
Year :
GLP : no data
Test substance : other TS: radiolabeled (14C) DIDP in acetone
Remark : 5 to 50 ug/L nominal concentrations; 4.4 to 41.7 ug/L mean measured concentrations. Chemical and radiochemical purity > 97.5%.
BCF based on wet weight.
BCF is based on total radioactivity (parent compound and

metabolites) and may significantly overestimate the extent to which DIDP parent is bioconcentrated.
Depuration half-life approximately 3.5 days.
No apparent adverse effects observed.

21.03.1996 (15)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Cyprinodon variegatus (Fish, estuary, marine)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .47 -
LC50	:	> .47 -
Method	:	other: see remarks
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	LC50 and NOEC determinations were limited by DIDP solubility. No acute effects observed at highest concentration tested. Procedure followed U.S. Environmental Protection Agency (1975) and complied with OECD Guidelines.

20.03.1996 (31)

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .62 -
LC50	:	> .62 -
Method	:	other: see remarks
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	LC50 and NOEC determinations were limited by DIDP solubility. No acute effects observed at highest concentration tested. Procedure followed U.S. Environmental Protection Agency (1975) and complied with OECD Guidelines.

20.03.1996 (31)

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> 1 -
LC50	:	> 1 -
Method	:	other: see remarks
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	LC50 and NOEC determinations were limited by DIDP solubility. No acute effects were observed at the highest concentration tested. Procedure followed U.S. Environmental Protection Agency (1975) and complied with OECD Guidelines.

20.03.1996 (31)

Type	:	semistatic
Species	:	other: Rana arvalis (Moorfrog)
Exposure period	:	28 day

Unit	:	mg/kg soil dw
Analytical monitoring	:	
NOEC	:	>= 600 -
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	ExxonMobil Biomedical Sciences, Inc.

05.06.2001 (125)

Type	:	static
Species	:	Lepomis macrochirus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .37 -
LC50	:	> .37 -
Method	:	other: procedure followed U.S. Environmental Protection Agency (1975) and complied with OECD Guidelines
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	LC50 and NOEC determinations were limited by DIDP solubility. No acute effects observed at highest concentration tested. Recalculated data from CMA Phthalate Esters Panel. Summary Report - Environmental Studies - Phase I. Generation of Environmental Fate and Effects Data Base on 14 Phthalate Esters. Chemical Manufacturers Association, Washington, DC. December 15, 1984.

20.03.1996 (5)

Type	:	static
Species	:	Lepomis macrochirus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .55 -
LC50	:	> .55 -
Method	:	other: see remarks
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	LC50 and NOEC determinations were limited by DIDP solubility. No acute effects were observed at the highest concentration tested. Procedure followed U.S. Environmental Protection Agency (1975) and complied with OECD Guidelines.

20.03.1996 (31)

Type	:	static
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
LC50	:	> 1 -
Method	:	other
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The test was a 96 hour aerated static test. Ten fish were used per test concentration, and the test was carried out at

15 +/- 1 degree C.

20.03.1996 (63)

Type	:	static
Species	:	Oryzias latipes (Fish, fresh water)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no data
LC50	:	> 3000 -
Method	:	other: Japanese Industrial Standard (JIS K 0102-1986-71) "Testing Methods for Industrial Waste Water"
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Exposure concentrations tested represent emulsions of undissolved DIDP.

21.03.1996 (28)

Type	:	static
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .47 -
LC50	:	> .47 -
Method	:	other: see remarks
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	LC50 and NOEC determinations were limited by DIDP solubility. No acute effects observed at highest concentration tested. Procedure followed U.S. Environmental Protection Agency (1975) and complied with OECD Guidelines. Recalculated data from CMA Phthalate Esters Panel. Summary Report - Environmental Studies - Phase I. Generation of Environmental Fate and Effects Data Base on 14 Phthalate Esters. Chemical Manufacturers Association, Washington, D.C. December 15, 1984.

20.03.1996 (6)

Type	:	static
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .66 -
LC50	:	> .66 -
Method	:	other: see remarks
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	LC50 and NOEC determinations were limited by DIDP solubility. No acute effects were observed at the highest concentration tested. Procedure followed U.S. Environmental Protection Agency recommendations (1975) and complied with OECD Guidelines.

20.03.1996 (31)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	µg/l
Analytical monitoring	:	yes
EC50	:	> 320 -
Method	:	OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year	:	1981
GLP	:	no data
Test substance	:	other TS: DIDP radiolabeled with 14C. Chemical and radiochemical purity = 98%. Acetone carrier used.
Remark	:	Immobilization

20.09.1995 (14)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no data
EC50	:	> 1 -
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

20.09.1995 (78)

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	= 1 -
LC50	:	> 1 -
Method	:	other: modified OECD Guideline 202
Year	:	1984
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Non-toxic dispersant used to minimize physical effects on daphnids that result when testing solutions containing undissolved DIDP.

23.05.2001 (16) (18)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	= .07 -
EC50	:	> .02 -
Method	:	other: see remark
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	EC50 determination was limited by DIDP solubility levels.[2] Procedure followed U.S. Environmental Agency (1975) and complied with OECD Guidelines. Recalculated data from CMA Phthalate Esters Panel. Summary Report - Environmental Studies - Phase I. Generation of Environmental Fate and Effects Data Base on 14 Phthalate

Esters. Chemical Manufacturers Association, Washington, D.C. December 15, 1984.

22.05.2001 (5)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .18 -
EC50	:	> .18 -
Method	:	other: see remarks
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	EC50 and NOEC determinations were limited by DIDP solubility. No acute effects observed at highest concentration tested. Procedure followed U.S. Environmental Protection Agency (1975) and complied with OECD Guidelines.

20.03.1996 (31)

Type	:	
Species	:	Mysidopsis bahia (Crustacea)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .08 -
LC50	:	> .08 -
Method	:	other: U.S. Environmental Protection Agency
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	LC50 and NOEC determinations were limited by DIDP solubility. No acute effects observed at highest concentration tested. Recalculated data from CMA Phthalate Esters Panel. Summary Report - Environmental Studies - Phase I. Generation of Environmental Fate and Effects Data Base on 14 Phthalate Esters. Chemical Manufacturers Association, Washington, D.C. December 15, 1984.

22.05.2001 (4)

Type	:	
Species	:	Mysidopsis bahia (Crustacea)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .15 -
LC50	:	> .15 -
Method	:	other: U.S. Environmental Protection Agency (1975)
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	LC50 and NOEC determinations were limited by DIDP solubility. No acute toxicity observed at highest concentration tested.

20.03.1996 (31)

Type	:	
Species	:	other: Paratanytarsus parthenogenica
Exposure period	:	96 hour(s)

Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .64 -
LC50	:	> .64 -
Method	:	other: U.S. Environmental Protection Agency (1975)
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	LC50 and NOEC determinations were limited by DIDP solubility. No acute toxicity observed at highest concentration tested. Recalculated data from CMA Phthalate Esters Panel. Summary Report - Environmental Studies - Phase I. Generation of Environmental Fate and Effects Data Base on 14 Phthalate Esters. Chemical Manufacturers Association, Washington, D.C. December 15, 1984.

22.05.2001 (5)

Type	:	other: sediment
Species	:	other: Chironomus tentans
Exposure period	:	10 day
Unit	:	mg/kg soil dw
Analytical monitoring	:	yes
NOEC	:	2630 -
Method	:	other: EPA/600/R-94/024
Year	:	1994
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Endpoints: survival and growth Tested at nominal concentration of 3000 mg/kg - dw of DIDP. No effect observed on survival or growth during the 10-day exposure.
Source	:	ExxonMobil Biomedical Sciences, Inc.
Reliability	:	(2) valid with restrictions

12.06.2001 (24)

Type	:	other: sediment
Species	:	other: Hyalella azteca
Exposure period	:	10 day
Unit	:	mg/kg soil dw
Analytical monitoring	:	yes
NOEC	:	2090 -
Method	:	other: EPA/600/R-94/024
Year	:	1994
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Endpoints: survival and growth Tested at nominal concentration of 3000 mg/kg - dw of DIDP. No effects observed on survival or growth during the 10-day exposure.
Source	:	ExxonMobil Biomedical Sciences, Inc.
Reliability	:	(2) valid with restrictions

12.06.2001 (24)

Type	:	
Species	:	other: Paratanytarsus parthenogenica
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .96 -
LC50	:	> .96 -
Method	:	other: see remarks
Year	:	1975
GLP	:	yes

Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	LC50 and NOEC determinations were limited by DIDP solubility. No acute toxicity observed at highest concentration tested. Method: U.S. Environmental Protection Agency (1975).

20.03.1996 (31)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	growth rate
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> 1.3 -
EC50	:	> 1.3 -
Method	:	other: procedure followed U.S. Environmental Protection Agency (1975) and complied with OECD Guidelines
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	EC50 and NOEC determinations were limited by DIDP solubility. No acute toxicity observed at highest concentration tested.

20.03.1996 (31)

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	growth rate
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	> .8 -
EC50	:	> .8 -
Method	:	other: see remarks
Year	:	1975
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	EC50 and NOEC determinations were limited by DIDP solubility. No acute toxicity observed at highest concentration tested. Procedure followed U.S. Environmental Protection Agency (1975) and complied with OECD Guidelines. Recalculated data from CMA Phthalate Esters Panel. Summary Report - Environmental Studies - Phase I. Generation of Environmental Fate and Effects Data Base on 14 Phthalate Esters. Chemical Manufacturers Association, Washington, D.C. December 15, 1984.

20.03.1996 (5)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type	:	aquatic
Species	:	activated sludge of a predominantly domestic sewage
Exposure period	:	3 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC0	:	> 100 -

Method : other: Procedures generally followed OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test." (See remarks section)
Year :
GLP : yes
Test substance :
Remark : Methods cont'd.--However, oxygen consumption was determined using an automated electrolytic respirometer rather than a dissolved oxygen probe. Due to the increased sensitivity of this instrument in determining oxygen uptake, a lower sludge loading (30 mg/l) than prescribed in the OECD Guideline was also used.
This toxicity test was conducted as a "Limit Test." A nominal concentration of 100 mg/l TS was prepared in mineral water contained in a glass vessel that included a teflon stir bar. The vessel was then placed on a stir plate and agitated for 24 hrs. A sample of the water accommodated fraction was then removed from a port at the bottom of this vessel for toxicity testing. Oxygen consumption by sewage sludge added to the water accommodated fraction was compared to control mineral water. Results indicated no inhibition of microbial respiration.

22.05.2001 (41)

Type : aquatic
Species : activated sludge, domestic
Exposure period : 30 minute(s)
Unit : mg/l
Analytical monitoring : yes
EC0 : = 83 -
Method : OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year : 1984
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : A stock solution was prepared using a 1:10 ratio of test substance: Tween 20 dispersant.
Source : ExxonMobil Biomedical Sciences, Inc.

12.06.2001 (43)

Type : aquatic
Species : Photobacterium phosphoreum (Bacteria)
Exposure period : 15 minute(s)
Unit : mg/l
Analytical monitoring : yes
EC0 : = 83 -
Method : other
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : A stock solution was prepared using a 1:10 ratio of test substance: Tween 20 dispersant.
Source : ExxonMobil Biomedical Sciences, Inc.

12.06.2001 (44)

Type : aquatic
Species : Photobacterium phosphoreum (Bacteria)
Exposure period : 15 minute(s)
Unit : mg/l
Analytical monitoring : no
EC0 : > 100 -
Method : other: See remarks section)
Year :
GLP : yes

Test substance :
Remark : Method--A nominal concentration of 100 mg/l TS was prepared in lab dilution water contained in a glass vessel that included a teflon stir bar. The vessel was then placed on a stir plate and agitated for 24 hrs. A sample of the water accommodated fraction was then removed from a port at the bottom of this vessel for microtox testing. Serial dilutions representing 100%, 50%, 25%, 12.5% and 6.25% of the original water accommodated solution were prepared and assayed with microtox according to procedures specified by the manufacturer.
Results indicated no inhibition of Photobacterium phosphoreum light production for all treatments investigated.

22.05.2001 (41)

4.5.1 CHRONIC TOXICITY TO FISH

Species : Oryzias latipes (Fish, fresh water)
Endpoint :
Exposure period : 284 day
Unit :
Analytical monitoring : yes
Method :
Year : 2001
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : Test substance was tested in a multi-generation dietary exposure protocol to evaluate reproductive and developmental effects in the Japanes Medaka. Test substance was spiked via an acetone solution into a fish flake food at 20µg/g. Fish were fed at a daily rate of 5% body weight / day. Fo and F1 generation adults were reared through sexual maturation and ovipositor (140 days-post-hatch). Test ended with F2 generation prior to sexual maturation.

Effects were evaluated using population, individual, and biochemical parameters including: survival, sex ratio, fecundity, development, growth, gonadal-somatic index, histopathology,
testosterone metabolism, EROD activity, and vitellogenin production.

Results indicated that egg production was similar among all treatment groups. F1 and F2 generation embryos showed normal development except for transient change in red blood cell pigmentation in the phthalate and acetone groups. There were no treatment-related alterations in survival, fecundity, or GSI and no histological lesions were observed.

There was no shift in male-to-female ratio and the phenotypic and histological gender classifications for both male and female fish were in agreement. Testosterone metabolism, EROD activity, and vitellogenin levels were not significantly different among treatment groups.
Source : ExxonMobil Biomedical Sciences, Inc.
Reliability : (1) valid without restriction
12.06.2001 (99)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species : Daphnia magna (Crustacea)
Endpoint : other: mortality and reproduction rate

Exposure period : 21 day
Unit : mg/l
Analytical monitoring : yes
NOEC : = .03 -
LCEC : = .06 -
Method : other: procedures developed by Springborn Laboratories
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Daphnids observed at surface of test solution at LOEC.
Physical effects (e.g. surface entrapment) caused by direct exposure to undissolved DIDP are likely responsible for the daphnid immobilization.
Geometric mean maximum acceptable toxicant concentration (MATC) = 0.042.
Highest mean measured concentration = 0.14 mg/L.
Observed chronic toxicity appeared to be due to surface entrapment.
Recalculated data from CMA Phthalate Esters Panel. Summary Report - Environmental Studies - Phase I. Generation of Environmental Fate and Effects Data Base on 14 Phthalate Esters. Chemical Manufacturers Association, Washington, D.C. December 15, 1984.
Survival is more sensitive as an endpoint than reproduction.

22.05.2001 (105)

Species : Daphnia magna (Crustacea)
Endpoint : other: parent and offspring survival, growth (parent length), reproduction
Exposure period : 21 day
Unit : mg/l
Analytical monitoring : yes
NOEC : = 1 -
Method : other: Modified OECD Guide-line 202
Year : 1984
GLP : yes
Test substance : other TS: as prescribed by 1.1 - 1.4 dispersed with caster oil ethoxylate
Remark : A non-toxic dispersant was used to minimize physical effects which may result when testing solutions containing of undissolved DIDP.
There were no significant effects relative to the control in terms of parent daphnia size, numbers of young/parent or survival of offspring exposed to a nominal concentration of 1 mg/l DIDP.

04.06.2001 (19) (34)

Species : Daphnia magna (Crustacea)
Endpoint : other: parent survival; parent length; numbers of offspring; offspring survival
Exposure period : 21 day
Unit : mg/l
Analytical monitoring : yes
Method : other: modified OECD Guideline 202, Part II
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : COE alone had an influence on parental survival (> or = 30% mortality). There were no significant effects related to control in terms of parent Daphnia size (at 21 days),
numbers of young/surviving parent Daphnia or survival of offspring exposed to a nominal DIDP concentration of 1 mg/L in 10 mg/L of COE.
No mortality and insignificant flotation at a nominal DIDP

concentration of 1 mg/L (measured 0.86 mg/L) in 10 mg/L of COE.
Non-toxic dispersant used to minimize physical effects on daphnids that result when testing solutions containing emulsions of undissolved test chemical.

04.06.2001 (17)

Species	:	Daphnia magna (Crustacea)
Endpoint	:	other: see remark
Exposure period	:	21 day
Unit	:	µg/l
Analytical monitoring	:	yes
NOEC	:	> 100 -
Method	:	other: OECD Guideline 202, part 1
Year	:	1981
GLP	:	no data
Test substance	:	other TS: 14C radiolabeled DIDP in acetone; chemical and radiochemical purity was 98%
Remark	:	DIDP had no effect on reproduction at nominal concentrations up to and including 100 ug/l.

03.11.1995 (14)

Species	:	other: Chironomus riparius
Endpoint	:	other: survival and development and emergence; see remarks
Exposure period	:	28 day
Unit	:	mg/kg soil dw
Analytical monitoring	:	yes
NOEC	:	>= 10000 -
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: C14 labeled DIDP (radiochemical purity >= 91.4%)
Remark	:	Endpoints: Time to first emergence; time to 50% emergence; emergence after 28 days; sex distribution. Larvae (< 24 hours posthatch) tested. No adverse effects were observed from first larval stage to emergence at any of the concentrations tested. River sediment was spiked with DIDP at three concentrations: 100, 1000 and 10,000 mg phthalate/kg (dry weight).

22.05.2001 (21)

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

Species	:	Raphanus sativus (Dicotyledon)
Endpoint	:	other: see remark
Exposure period	:	
Unit	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: unspecified DIDP
Remark	:	Diisodecyl phthalate produced no damage to test plants exposed to an air stream containing DIDP. Air concentration of DIDP not specified. Photosynthesis and respiration were measured.

21.03.1996 (52)

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	Wistar
Sex	:	male
Number of animals	:	5
Vehicle	:	
Value	:	> 60000 - mg/kg bw
Method	:	other: Smyth H.F. et al. Am. Ind. Hyg. Assoc. J. 23:95-107
Year	:	1962
GLP	:	no data
Test substance	:	other TS: unspecified DIDP isomer
Remark	:	DIDP was administered to groups of 5 non-fasted Wistar male rats by gastric intubation. A 14 day observation period was used.
Result	:	In a series of acute toxicity tests in rats, no lethality was reported up to 29,100 mg/kg. No clinical signs or macroscopic changes were observed at 15,00 mg/kg. Diarrhea and loss of weight were observed at 29,1000 mg/kg. The LD50 of DIDP in rats is greater than 62,080 mg/kg.
Reliability	:	(4) not assignable

18.05.2001 (116)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 64000 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: unspecified DIDP
Remark	:	Protocol not specified.

17.03.1998 (114)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Species	:	laboratory animal
Strain	:	other
Sex	:	male/female
Number of animals	:	30
Vehicle	:	
Exposure time	:	6 hour(s)
Value	:	> .13 - mg/l
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A 6-hour exposure inhalation study was conducted in rats, mice and guinea pigs (5 males and 5 females) at 0.13 mg/l (nominal concentration)vapor concentration. Following an 14-day observation period, no deaths occurred, no signs of

toxicity, or respiratory tract irritation and no gross pathological lesions were seen.

The test concentration of this study was low due to the fact that DIDP has a very low vapor pressure. Therefore, DIDP is unlikely to be hazardous by inhalation.

01.06.2001 (3)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	male
Number of animals	:	
Vehicle	:	
Value	:	= 16000 - mg/kg bw
Method	:	other: Smyth H.F. et al. Am. Ind. Hyg. Assoc. J. 23:95-107
Year	:	1962
GLP	:	no
Test substance	:	other TS: unspecified DIDP
Remark	:	A single 24-hour application of undiluted DIDP was applied to intact rabbit skin (n = 4). A 14 day observation period was used.

18.05.2001 (116)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 3160 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A single 24-hour application of undiluted DIDP (200 and 3160 mg/kg) was applied to abraded rabbit skin under occlusive covering (n = 4). A 14 day observation period was used.

18.03.1996 (2)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	4
Vehicle	:	
Value	:	> 3160 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A single 24-hour dermal exposure of undiluted DIDP was applied to the abraded skin of rabbits (4 animals, sex not specified).

18.05.2001 (1)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	i.p.
Exposure time	:	168 hour(s)
Method	:	other : not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: DIDP with different CAS#
Remark	:	LD50 >100 g/kg. No deaths were observed. Mice (n = 10) were administered undiluted DIDP i.p. and observed for 7 days.

23.02.1998 (75)

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	.5 other: ml
Exposure	:	Semiocclusive
Exposure time	:	60 minute(s)
Number of animals	:	6
PDII	:	0
Result	:	not irritating
EC classification	:	not irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1992
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Six male rabbits were exposed to 0.5 ml of the test material during 4 hours. The patch was held in contact with the skin by means of a semi-occlusive dressing. Only very slight erythema in one animal was noted at 60 minutes after removal of the patch, no other signs of irritation were noted.
Reliability	:	(1) valid without restriction

21.05.2001 (104)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	slightly irritating
EC classification	:	not irritating
Method	:	other: 24 hr exposure
Year	:	
GLP	:	no data
Test substance	:	other TS: unspecified DIDP
Remark	:	A single 24-hour application of undiluted DIDP was applied to the intact skin of rabbits.

18.05.2001 (116)

Species	:	human
Concentration	:	100 %
Exposure	:	Occlusive
Exposure time	:	24 hour(s)
Number of animals	:	104
PDII	:	0

Result	:	not irritating
EC classification	:	not irritating
Method	:	other: single 24 hr application
Year	:	1999
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	DIDP was administered to human volunteers via a single 24-hour occluded patch application. Evaluations were made at 30 minutes and 24 hours after patch removal. No dermal responses were observed. The group mean irritation score was 0.00.

18.05.2001 (87)

Species	:	mouse
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	10
PDII	:	
Result	:	not irritating
EC classification	:	not irritating
Method	:	other: single intradermal injection
Year	:	
GLP	:	no data
Test substance	:	other TS: DIDP with different CAS#
Remark	:	Protocol not specified. A study using Lawrence's method was conducted on 10 mice: undiluted DIDP produced no signs of irritation.

18.05.2001 (75)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	.1 undiluted
Dose	:	.1 ml
Exposure Time	:	
Comment	:	
Number of animals	:	6
Result	:	slightly irritating
EC classification	:	not irritating
Method	:	Draize Test
Year	:	1975
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	0.1 ml of undiluted DIDP was applied into the conjunctival sac of six rabbits. Scoring for irritation was carried out after 1, 4, 24, 48 and 72 hours, and 7 days. Undiluted DIDP produced only slight signs of irritation in the conjunctiva at 1, 4 and 24-hours. All the eyes were normal at 48, 72 and 96 hours.

18.05.2001 (48)

Species	:	rabbit
Concentration	:	undiluted
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	not irritating

EC classification	:	not irritating
Method	:	other: Lawrence W.H. et al. J.Pharm.Sci. 60:568-571.
Year	:	
GLP	:	no data
Test substance	:	other TS: DIDP with different CAS#
Remark	:	Protocol not specified. In a study for which minimal experimental details were provided, undiluted DIDP did not produce any obvious irritation.

21.05.2001 (75)

5.3 SENSITIZATION

Type	:	Buehler Test
Species	:	guinea pig
Concentration	:	Induction undiluted occlusive epicutaneous Challenge 5 % occlusive epicutaneous Challenge 1 % occlusive epicutaneous
Number of animals	:	40
Vehicle	:	Peanut Oil
Result	:	ambiguous
Classification	:	sensitizing
Method	:	OECD Guide-line 406 "Skin Sensitization"
Year	:	1981
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Observations inconsistent with typical sensitization reactions. In a modified Buehler test, 40 guinea pigs (20 treated females and 20 controls) were used for the assessment of dermal sensitization. Induction phase; was performed on days 0, 7 and 14 by occlusive topical application with undiluted DIDP.

21.05.2001 (36)

Type	:	Buehler Test
Species	:	guinea pig
Concentration	:	Induction undiluted Challenge undiluted
Number of animals	:	40
Vehicle	:	
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	other: Directive 92/69/EEC, B.6
Year	:	1992
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	In a Buehler test undiluted DINP was applied to 40 guinea-pigs (20 treated and 20 controls). No signs of sensitization or irritation were noted in any of the animals.

01.06.2001 (71)

Type	:	Patch-Test
Species	:	human
Concentration	:	Induction 100 % occlusive epicutaneous Challenge 100 % occlusive epicutaneous
Number of animals	:	104

Vehicle	:	
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	other: Modified Draize Patch Test
Year	:	1999
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Isolated case reports suggest that dermal contact with some phthalate esters may result in skin sensitization. Consequently, 7 dialkyl phthalate esters, ranging in carbon number C6 to C13, were tested in a 104-person panel (Human Repeated Insult Patch Test HRIPT) using the modified Draize procedure. Test concentrations of 100% were selected for the induction and challenge phases of the HRIPT based upon a 24-h occluded irritation test on 15 panelists. Under the conditions of this HRIPT, no evidence of dermal irritation or sensitization of any of these 7-phthalate esters was observed in any of the 104 panelists. These HRIPT data provided evidence of the lack of experimental skin sensitization potential for the phthalate esters tested. DIDP was tested at a 100% concentration for both induction and challenge phases. The induction phase involved application 3X/week for 3 weeks. The challenge dose was applied after a 10 - 17 day rest period. There were no skin reactions and no evidence of either cumulative irritation or sensitization.
Result	:	Of the 128 panelist enrolled in the HRIPT, 104 completed the study; the remainder did not complete the study for reasons unrelated to the test materials. During both induction and challenge phases of the study, there was no evidence of dermal irritation.
Conclusion	:	Under the conditions of the HRIPT, there was no evidence of skin irritation or sensitization in any of the 104 panelists completing the study. These HRIPT data provided evidence for the lack of skin sensitization potential for diisodecyl phthalate in humans.

01.06.2001 (88)

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	21 days
Frequency of treatment	:	daily
Post obs. period	:	no
Doses	:	0.3, 1.2, 2.5% (approx. 280, 1100, and 2000 mg/kg/day)
Control group	:	yes, concurrent no treatment
NOAEL	:	ca. 280 - mg/kg bw
LOAEL	:	ca. 1100 - mg/kg bw
Method	:	other: not specified
Year	:	1986
GLP	:	yes
Test substance	:	other TS: DIDP with different CAS#
Result	:	Absolute and relative LIVER WEIGHTS and relative KIDNEY WEIGHTS were INCREASED in animals given 1.2 or 2.5% DIDP. Both sexes given 2.5% DIDP showed INCREASES IN PEROXISOME NUMBERS AND SIZE, with the females showing a greater response. INCREASES IN PALMITOYL CoA OXIDATION and TOTAL HEPATIC PROTEIN LEVELS were also observed at these doses.

04.06.2001 (9)

Species	:	rat
Sex	:	male/female
Strain	:	other: Charles River Caesarean-derived
Route of admin.	:	oral feed
Exposure period	:	13 weeks
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	0.05, 0.3, 1% (approx. 25, 150 and 500 mg/kg/day)
Control group	:	yes, concurrent no treatment
NOAEL	:	ca. 150 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: unspecified DIDP
Remark	:	10 rats/sex/group were exposed to 0.05, 0.3 and 1% DIDP in feed for 13 weeks. Criteria for evaluation of a compound effect were physical appearance, behavior, growth, food consumption, survival, clinical laboratory values, organ weights, and gross and microscopic pathology.
Result	:	No compound related effects were observed at any dietary levels with regard to physical appearance, behavior and survival. Body weight gains for the two higher levels in the males were lower than the controls, but not significantly different. Body weight gains for the high level females were only slightly lower than the controls. Observations at necropsy revealed increased liver weights in the high dose animals. No other changes were observed.

21.05.2001 (37) (114)

Species	:	dog
Sex	:	male/female
Strain	:	Beagle
Route of admin.	:	oral feed
Exposure period	:	13 weeks
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	0.05, 0.3, 1% (approx. 15, 75 and 300 mg/kg/day)
Control group	:	yes, concurrent no treatment
NOAEL	:	ca. 75 - mg/kg bw
LOAEL	:	ca. 250 - mg/kg bw
Method	:	other: not specified
Year	:	1973
GLP	:	no data
Test substance	:	other TS: unspecified DIDP
Remark	:	3 dogs/sex/group were exposed to 0.05, 0.3 and 1% DIDP in feed for 13 weeks. Criteria for evaluation of a compound effect were physical appearance, behavior, growth, food consumption, survival, clinical laboratory values, organ weights, and gross and microscopic pathology.
Result	:	All treated groups and controls appeared normal with respect to appearance, behavior and elimination. Three dogs in the highest diet level showed slight to moderate body weight losses, these findings did not appear to be related to decreased food consumption except for one animal. All clinical laboratory values were generally within acceptable limits and comparable between all groups. Gross necropsy examinations did not reveal any consistent compound-related alterations. At the high dose a SLIGHTLY ELEVATED LIVER/BODY WEIGHT RATIO was noted in all males and 2/3 of females.

Pathological examination revealed SWOLLEN AND VACUOLATED HEPATOCYTES in the livers of these animals. No other histological changes were observed.

21.05.2001 (114) (122)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella strains TA98, TA100, TA1535, TA1537
Concentration : up to 10 mg/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: Ames BN et al. Mutat Res. 31:347-364.
Year : 1975
GLP : no data
Test substance : other TS: DIDP with different CAS#
Remark : Standard plate and preincubation test both with and without metabolic activation (Aroclor induced rat or hamster liver S-9). DIDP was tested at 5 dose levels separated by half-log intervals.

23.02.1998 (129) (130)

Type : Mouse lymphoma assay
System of testing : TK locus of mouse lymphoma cells, L5178Y cell line
Concentration : 0.25 to 10 ul/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: not specified
Year :
GLP : yes
Test substance : other TS: unspecified DIDP
Remark : There was no indication of mutagenic potential for DIDP in the mouse lymphoma assay.
Conclusion : The data presented in this report confirm the general lack of genotoxicity for DIDP. Phthalate esters do not contain substructures that would be considered 'alerting' for mutagenicity.

01.06.2001 (8) (55)

Type : other: 8-azaguanine resistance assay
System of testing : Salmonella typhimurium strain TA100
Concentration : no data
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: Skopek et al. Proc. Natl. Acad. Sci. 75:410-414,4465-4469
Year : 1978
GLP : no data
Test substance : other TS: DIDP with a different CAS#
Remark : Assay was conducted in a liquid suspension and bacteria were tested for mutation to 8-azaguanine resistance. No increase in mutant frequency was observed at any concentration of DIDP.

04.06.2001 (113)

Type : other: cell transformation assay
System of testing : BALB/C-3T3 mouse cell line cells, L5178Y cell line
Concentration : 0.2 to 20 ul/ml
Cycotoxic conc. :
Metabolic activation : without

Result	:	negative
Method	:	other: not specified
Year	:	
GLP	:	yes
Test substance	:	other TS: unspecified DIDP

21.05.2001 (8) (81)

Type	:	other: cell transformation assay
System of testing	:	BALB/C-3T3 cells
Concentration	:	0, 0.01, 0.1 and 1.0 ug/ml
Cycotoxic conc.	:	
Metabolic activation	:	without
Result	:	positive
Method	:	other: not specified
Year	:	
GLP	:	yes
Test substance	:	other TS: unspecified DIDP
Remark	:	DIDP produced significantly greater transformation frequencies at 1.0 ug/ml.

23.02.1998 (90)

5.6 GENETIC TOXICITY 'IN VITRO'

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	CD-1
Route of admin.	:	gavage
Exposure period	:	24, 48, and 72 hours
Doses	:	1250, 2500, and 5000 mg/kg
Result	:	negative
Method	:	other: modification of Heddle et a. Mutat. Res. 123:61-118.
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	DIDP was inactive in an in vivo micronucleus test. There were no significant differences between treatment groups and controls for either male or female mice at any dose or collection time.
Conclusion	:	No Clastogenic effects in bone marrow.

21.05.2001 (85) (93)

5.7 CARCINOGENITY

5.8 TOXICITY TO REPRODUCTION

Type	:	Two generation study
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	premating through post-partum of both generations
Frequency of treatment	:	continuous (diet)
Premating exposure period		
Male	:	10 weeks, 7 weeks old
Female	:	10 weeks, 7 weeks old

Duration of test	:	19 weeks, both generations
Doses	:	In the first study 0.2, 0.4, 0.8% were target dietary concentrations, 30/sex/group. In the second study the target concentrations were 0.02%, 0.06%, 0.2%, and 0.4% in diet, 30/sex/group.
Control group	:	yes, concurrent no treatment
NOAEL Parental	:	= 600 - mg/kg bw
NOAEL F1 Offspr.	:	= 600 - mg/kg bw
NOAEL F2 Offspr.	:	= .06 - %
other	:	= .8 - %
Method	:	Directive 87/302/EEC, part B, p. 47 "Two-generation reproduction toxicity test"
Year	:	2000
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	In the reproductive studies, there were no effects on fertility or on live birth index and no effects on testicular development. Overall, these studies defined No-Observed-Adverse-Effect Levels (NOAELs) of 0.06% (approximately 50 mg/kg/day) for F2 offspring survival and 0.8% (approximately 600 mg/kg/day) for fertility, other measures of reproductive function, and developmental landmarks. Statistical evaluation of the data from both studies identified 108 mg/kg/day with a 95% lower bound value of 86 mg/kg/day as a theoretical NOAEL for reduced F2 offspring survival.
Result	:	No-Observed-Adverse-Effect Levels (NOAELs) for fertility was 0.8%, and for offspring survival was 0.06% (F2 gen, PND 1-4). There were no important or dose-dependent clinical signs of toxicity in either the P1 males or females in any dose group. There were no treatment-related deaths or gross postmortem observations judged to have been related directly to treatment with the test material in any P1 or F1 animals. Increased liver and kidney weights were found at all dose levels in male and female adults. There were no differences observed in mating, male or female fertility, gestational index, or length of gestation. Furthermore, there were no differences in mean litter size or sex ratio. The percentage of live offspring was significantly decreased in the 0.8% dose group and below the laboratory historical control range (HCR). In addition, reduced offspring survival was observed at postnatal days 1 and 4 in the F2 generation (but not in the F1 generation) at levels of 0.2% DIDP and greater. There was a statistically significant increase in age of vaginal patency in the 0.4 and 0.8% dose groups, but overall the differences were small (approximately 2 days) and within the range of unknown biologic relevance. No clinical signs of toxicity or gross postmortem observations were noted in the offspring. There were no differences in viability at weaning during the postnatal period. There were no differences in F1 offspring developmental landmarks, anogenital distance, nipple retention, preputial separation, or vaginal patency. There were no differences in testicular weights in either parents (P1) or offspring (F1) and there were no pathological changes in the testes. Further, there were no differences in offspring body weight during the postnatal period to PND 35.
Conclusion	:	No overt changes in fertility, reproductive function or testicular development were observed. NOAELs for fertility and reproductive development were approximately 1000 and 600 mg/kg/day based on the one and two generation studies respectively.
Reliability	:	(1) valid without restriction

10.09.2001 (60)

Type	:	other: Investigation of testicular atrophy
Species	:	rat
Sex	:	male
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	28 days
Frequency of treatment	:	daily
Premating exposure period		
Male	:	
Female	:	
Duration of test	:	
Doses	:	
Control group	:	
Remark	:	DIDP was given by dietary administration for 28 days to juvenile male F-344 rats. Dietary levels were 0.02, 0.05, 0.10, 0.30 and 1.0%; the highest dietary level was equivalent to 1287 mg/kg/day. Based on histological changes and organ weight data, DIDP did not induce testicular atrophy in this study. Thus, the NOAEL was 1287 mg/kg/day, the highest dose tested.

21.05.2001 (12) (74)

Type	:	other: Testicular atrophy
Species	:	rat
Sex	:	male
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	21 days
Frequency of treatment	:	daily
Premating exposure period		
Male	:	
Female	:	
Duration of test	:	
Doses	:	
Control group	:	
Remark	:	DIDP was administered in the diet for 21 days to juvenile male F-344 rats. Dietary levels were 0.3, 1.2 and 2.5% corresponding to approximately 304, 1134,and 2100 mg/kg/day. DIDP did not produce testicular atrophy in this study. The NOAEL was 2100 mg/kg/day, the highest dose tested.

21.05.2001 (11) (79)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Gd 6 through 15
Frequency of treatment	:	daily
Duration of test	:	gestation day 21
Doses	:	100, 500, 1000 mg/kg
Control group	:	yes, concurrent vehicle
NOAEL Maternalt.	:	500 - mg/kg bw
NOAEL Teratogen	:	1000 - mg/kg bw

Method	:	Directive 87/302/EEC, part B, p. 24 "Teratogenicity test - rodent and non-rodent"
Year	:	1981
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The result indicate that DIDP was neither a selective developmental toxicant nor an embryotoxic agent.
Result	:	Maternal toxicity was indicated by reductions in body weight gain and food consumption. There was no evidence of malformations or fetal toxicity.
Reliability	:	(1) valid without restriction
04.06.2001		(95) (123)

Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	day 6-15 of gestation
Frequency of treatment	:	daily
Duration of test	:	day 20 of gestation
Doses	:	40, 200, 1000 mg/kg/day
Control group	:	yes, concurrent vehicle
NOAEL Maternalt.	:	= 200 -
NOAEL Teratogen	:	= 200 -
Method	:	Directive 87/302/EEC, part B, p. 24 "Teratogenicity test - rodent and non-rodent"
Year	:	1987
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A statistically significant increase in relative kidney and liver weights noted in the 1000 mg/kg/day dams. The only fetal effects were an increased occurrence of fetal skeletal variations consisting mainly of rudimentary cervical and/or accessory 14th rib(s) in the 1000 mg/kg/day group.
Reliability	:	(2) valid with restrictions
04.06.2001		(56)

Species	:	mouse
Sex	:	female
Strain	:	CD-1
Route of admin.	:	gavage
Exposure period	:	gestation days 6-13
Frequency of treatment	:	daily
Duration of test	:	
Doses	:	9650 mg/kg/day
Control group	:	yes
NOAEL Maternalt.	:	> 9650 - mg/kg bw
NOAEL Teratogen	:	> 9650 - mg/kg bw
Method	:	Directive 87/302/EEC, part B, p. 24 "Teratogenicity test - rodent and non-rodent"
Year	:	1987
GLP	:	yes
Test substance	:	other TS: DIDP with different CAS #.
Reliability	:	(1) valid without restriction
04.06.2001		(53)

5.10 OTHER RELEVANT INFORMATION

Type	:	Metabolism

Remark : The fate of di-isodecyl phthalate (DIDP) was evaluated in male Sprague Dawley rats (3/exposure) ingesting (14C) DIDP via gavage at single doses of 0.1, 11.2 or 1000 mg/kg. After treatment, animals were placed in metabolism cages and feces was collected at 24 hour intervals and urine was collected at 12 hour intervals for a 72 hour period. At the end of the collection period, all animals were sacrificed and selected tissue was excised for analysis. 99% of the administered dose was recovered in the excreta for all dose levels. The primary route of elimination of radioactivity was via the feces, accounting for 58, 66 and 82% of the administered dose for low-, mid- and high-dose animals, respectively. HPLC analysis of the fecal extract revealed that 30% of the radioactivity at the low dose and 60% at the high dose were of the parent compound. Excretion in the urine was biphasic and no apparent dose related effect on the rates of elimination was detected. Urine metabolites identified were phthalic acid, accounting for 38, 48 and 18% of the radioactivity in the urine from low-, mid- and high-dose animals, respectively and the remainder as mono-isodecyl phthalate derivatives.

22.05.2001 (50)

Type : Metabolism
Remark : The fate of diisodecyl phthalate (DIDP) was evaluated in six male Sprague Dawley rats receiving head only exposure to 14C-DIDP at a nominal concentration of 100 mg/m(3) for six hours. Immediately following exposure, three animals were sacrificed and selected tissue was excised. The remaining animals were placed in Roth-type metabolism cages and feces were collected at 24 hour intervals and urine was collected at 12 hour intervals for 72 hours. At the end of the 72 hour collection period, animals were sacrificed and selected tissues were excised. Within the 72 hour test period, 86% of the total body burden was excreted in the urine (45% of the absorbed dose) and feces (41% of the absorbed dose) and 12% remained in the carcass. Urinary excretion was apparent first order with a half-life (T 1/2) of 16 hours. The highest concentration of radioactivity found in the organs of animals sacrificed immediately after exposure was the lung (mean value, 0.6630 +/- 0.2556u mole equivalents), followed by the gastro-intestinal tract (GIT) (mean value, 0.0948 +/- 0.0080u mole equivalents), liver (mean value, 0.0148 +/- 0.0012u mole equivalents) and kidney (mean value, 0.0064 +/- 0.0006u mole equivalents). Animals sacrificed 72 hours after exposure had only 27% of the original concentration remaining in the lungs and the concentration in the GIT, concentrations in liver and kidneys were reduced by 90%. The slow absorption of retained DIDP by the pulmonary tissue may be the rate limiting factor in its excretion.

22.05.2001 (51)

Type : other: Dermal Absorption and Excretion
Remark : A single dose (30 mg/kg) of 14C-labelled DIDP was dermally applied to male F344 rats. The rates of excretion (urine, feces) were calculated every 24 hours for 7 days. The amount of radioactivity in selected tissues was determined at 7 days. Only 0.5% of the applied dose was recovered in the feces and nothing was detected in the urine. Most of the remaining dose was recovered in the skin application area. These data indicate that DIDP is very poorly absorbed dermally.

22.05.2001 (39)

Type : other: Evidence of species differences in response based on in vitro studies

Remark : The effect of monoisodecyl phthalate (MIDP) on peroxisome proliferation was studied in primary monolayer cultures of rat and marmoset hepatocytes. Mono-(2-ethylhexyl) phthalate was used as a reference material, since it is the major phalate in in vivo metabolite of DEHP. Parameters examined were peroxisomal palmitoyl-CoA (PCoA) oxidation and laurate 11-and 12-hydroxylation (LAH). MIDP produced a marked
dose-related increase in PCoA oxidation of rat hepatocytes.

In addition, MIDP (at 2.5 mM) was less potent than MEHP (at 5 mM). In the marmoset hepatocytes only minimal changes with poor dose dependency were seen with MIDP, and no changes with MEHP. MIDP caused up to a thirteen-fold increase in LAH in rat hepatocytes and only up to a four-fold increase in marmoset hepatocytes. MEHP caused a six-fold increase in LAH in the rat cells but had no effect in marmoset hepatocytes. This marked species difference indicates caution should be used in extrapolating findings from rodent studies to man.

04.06.2001 (10)

Type : other: Evidence of species differences in response based on in vivo studies

Remark : The short term hepatic effects of DIDP were evaluated in rats and mice. When given to rats at 12000 ppm in the diet, evidence of peroxisomal proliferation including liver weight increases, elevated liver enzyme levels and elevated DNA synthesis were observed. None of these effects was altered when the rats were given 1000 ppm.

When given to mice at 6000 ppm in the diet, evidence of peroxisomal proliferation including liver weight increases, elevated liver enzyme levels and elevated DNA synthesis were observed. These parameters were not affected at 500 ppm in this study.

These data provide evidence that DIDP induces peroxisomal proliferation when given at high doses to rats and mice.

01.06.2001 (115)

Type : other: Inhibition of gap junctional intercellular communication in vitro

Remark : The comparative effects of several phthalate monoesters on inhibition of gap junctional intercellular communication (GJIC) and induction of peroxisomal beta-oxidation (PBox) were assessed in primary cultured hepatocytes from rats, mice, hamsters, Cynomolgus monkeys and humans. A human liver cell line was also utilized. Monoesters examined included mono-isodecyl phthalate (MIDP). GJIC was measured 4 and 24 hours after treatment with Lucifer yellow dye coupling. GJIC was inhibited in rat and mouse hepatocytes by MIDP in a dose-dependent manner and was substantially reversed within 24 hours of monoester removal. In contrast, cell-to-cell communication was not inhibited in hamster, cynomolgus or human hepatocytes or in a human liver cell line at any concentration examined. In rat and mouse hepatocytes PBox was elevated after treatment with MIDP, but there were no changes in PBOX levels in hepatocytes from other species. These data provide additional evidence that the toxicological effects of phthalate esters are species-specific.

04.06.2001 (72)

Type : other: Endocrine Disrupter

Remark : DIDP and a number of other comercially available phthalates were screened for estrogenic activity in a recombinant yeast assay. DIDP was

inactive in this test.
DIDP was tested in vitro for (a) estrogen receptor (ER) competitive ligand binding and (b) gene expression assays. DIDP was inactive in all of these in vitro assays.

DIDP was also tested for estrogenic activity in vivo using the uterotrophic assay/vaginal cornification assay: 20, 200, and 2000 mg/kg/day of DIDP were administered by oral gavage once daily for 4 days to ovariectomized Sprague-Dawley rats (10 females per dose, two experimental groups). Ethynyl estradiol (EE) was used as a positive control. Body weight, uterine wet weight and percentage of vaginal epithelial cell cornification were assessed on each day.

Neither DIDP nor any of the other phthalate esters tested produced a reproducible, dose-dependent effect on uterine wet weight relative to vehicle control at any of the doses tested. Additionally, none of the phthalate esters tested induced a significant vaginal cornification response at any of the doses tested.

04.06.2001 (54) (128)

5.11 EXPERIENCE WITH HUMAN EXPOSURE

Memo : Sources of General Exposure (air)
Remark : The levels of DIDP in air have been quantified in two publications. The first (Wechsler, 1984) measured aerosol collected from indoor and outdoor locations. The levels of DIDP in indoor air at two locations in the US were reported as 20 ng/m3. DIDP was not detectable in outdoor air. The second study (Tienpont et al., 2000) using a thermal desorption method, reported that levels of DIDP in air from both indoor and outdoor sources were below quantitation limits (20 ng/m3). Data from Oie et al. (1997) showing that DIDP is below detection limits in indoor suspended dust provide additional evidence that there is very little exposure to DIDP by inhalation.

04.06.2001 (98) (119) (124)

Memo : Sources of General Exposure (water)
Remark : DIDP has seldom been detected in either surface water or drinking water (see section 3.2). However, as a worst case assessment, a concentration equivalent to the water solubility limit can be used in exposure calculations. Careful experimental measurements and theoretical predictions reported in section 2.6 indicate that the water solubility of DIDP is < 1 ug/l. Assuming 2 liters of water are consumed per day, this yields a maximum exposure of 0.03 ug/kg/day for a 70 kg person.

04.06.2001

Memo : Sources of General Exposure (food)
Remark : The UK Ministry of Agriculture, Fisheries and Food (MAFF)Food Safety Directorate has carried out a survey of the levels of total and individual phthalates in samples of composite fatty foods from their Total Diet Study.

DIDP levels were reported as below detection limits in both food (MAFF, 1996a) and baby food (MAFF, 1996b; 1998).

Additionally, food samples of jam, pickles and sauces from containers with closed seals were analyzed during the late 1980s. DIDP was not detected in any sample at a detection limit of 1 mg/kg (N=10).

04.06.2001 (82) (83) (84) (91)

Memo : Urinary Metabolite Data
Remark : Using a novel and highly selective technique, monoester metabolites of seven commonly used phthalates were measured in urine samples from a reference population of 289 adult humans (Blount et al., 2000). This analytical approach allowed direct measurement of the individual phthalate metabolites while avoiding contamination form the parent diesters.

Although data on DIDP metabolites were not presented, the results of higher molecular weight phthalates including DEHP and DINP indicated that external exposures to these substances were even lower than had been predicted (David, 2000; Kohn et al., 2000). By analogy to the DEHP and DINP data, external exposures to DIDP are most likely less than 1 ug/kg/day.

Subsequent studies by the CDC with larger numbers of individuals (CDC, 2001) confirmed these initial findings.

01.06.2001 (13) (26) (35) (73)

Memo : Occupational exposure to DIDP

Remark : Limited monitoring data collected over several years to assess occupational exposure of process operations and maintenance technicians at a plasticizer plant indicate DIDP concentrations in air of <2 mg/m3. Assuming 10m3 of air is inhaled per working day, 220 working days per year, and 40 working years over a 70 year lifetime, the estimated occupational exposure for a 70 Kg individual is <100 ug/kg/day.

In another study (McKee, 2000) a limited study of DIDP exposure during production indicated that levels were below 30 ug/m3. A review of all of the monitoring data for DEHP, DINP and DIDP production indicated that exposures are normally very low (i.e., < 50 ug/m3), but that there are tasks including maintenance and possibly product sampling which may result in higher exposures for periods of relatively short duration.

Measurements during PVC production, although more limited, indicated that exposures were < 2 mg/m3.

Occupational Exposure 5.11.1

01.06.2001 (45) (86) (97)

Memo : Sources of General Exposure (occupation)

Remark : A recent monitoring study was performed at a Volkswagen processing plant in Germany that uses DINP and DEHP in product applications. DINP measurements were made in several locations that were expected to yield the highest workplace exposure concentrations. Results indicated DINP concentrations ranged from < 0.001 to 0.029 mg/m3. Similar concentrations were obtained for DEHP. Using the highest air concentration measured, a maximum DINP exposure of 1 ug/kg/day is obtained using the assumptions stated previously. Since the physiochemical properties and industrial uses of these phthalates are similar to DIDP, these data provide useful read across for assessing potential occupational exposure for DIDP.
As a worst case scenario, if the DIDP concentration in air is assumed to be at the highest occupational exposure limit of 10 mg/m3 identified in section 1.8, this translates into a maximum permissible exposure of 500 ug/kg/day using the assumptions stated previously.
Industrial hygiene surveys during 1983, 1986, 1988 and 1994 have been conducted at a plasticizer plant in the United States. Monitoring data indicate that DIDP concentrations are usually not observed above an analytical detection limit of approximately 0.05 mg/m3. This translates into a maximum exposure of 2.5 ug/kg/day using the assumptions stated previously. Results from these studies should be directly applicable to Europe since production facilities are operated similarly.

Since the physiochemical properties and industrial uses of di-2-ethylhexyl phthalate (DEHP) are very similar to DIDP, occupational exposure data for DEHP provides useful "read across" for DIDP. Several recent reviews indicate DEHP concentrations in workplace air range from <0.02 to a maximum value of 4.1 mg/m3. Based on the exposure assumptions described previously, estimated occupational exposure range from <1 to 210 ug/kg/day. CEFIC (1985) estimates occupational exposure to be 30-70 ug/kg/day.

04.06.2001 (7) (27) (59) (61) (66) (67) (68) (69) (70) (80) (121)

Memo : Estimates of exposure to DEHP

Remark : Independent estimates of the total daily intake of DEHP reported by various investigators are summarized below:

1 - 4 ug/kg/day CEFIC (1985)
5.8 ug/kg/day Canada (1993)
4 ug/kg/day ASTDR (1993)
0.1 - 0.5 ug/kg/day ECETOC (1994)

Limited data are availiable to estimate the total daily intake of DIDP through multiple exposure routes. However, exposure estimates reported for DEHP should provide a conservative "read across" to DIDP.
Multiple Exposure Routes

04.06.2001 (7) (25) (27) (38)

Memo : Estimates of exposure to total phthalates

Remark : In a recent study by Dutch Authorities, the total daily intake of "total" phthalates was estimated to be 7.3 ug/kg/day with an upperbound estimate of 21 ug/kg/day. If these estimates are weighted by relative production volume of the various phthalates to "total" phthalates, these estimates for exposure to DEHP and DIDP agree closely with exposure estimates provided above.

04.06.2001 (102)

04.06.2001

23.02.1998

04.06.2001

04.06.2001

01.06.2001

01.06.2001

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7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 111381-91-0
CAS No.	:	111381-91-0
TSCA Name	:	1,2-Benzenedicarboxylic acid, nonyl undecyl ester, branched and linear
Synonym	:	1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - high MW phthalates
Printing date	:	12.11.2001
Revision date	:	
Date of last Update	:	12.11.2001
Number of Pages	:	10
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers:
68648-93-1
117-84-0
68515-40-2
68515-45-7
68515-43-5
84-77-5
3648-20-2
85507-79-5
111381-91-0
68515-47-9

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to

their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

10.10.2001 (4)

2.5 PARTITION COEFFICIENT

Log pow	:	10.28 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (4)

2.6.1 WATER SOLUBILITY

Value	:	.00259 - other: ug/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

10.10.2001 (4)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.0000000000278 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (4)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	6.2 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (4)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.002
Water (level I)	:	0
Soil (level I)	:	97.8
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000

Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (3)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : other (calculation)
Year : 2000
Result : Soil - 97.8%
Air - 0.00204%
Water - 0.0000058%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (3)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Mouse lymphoma assay
System of testing	:	Mammalian cell
Concentration	:	0.125 to 6 ul/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year	:	2000
GLP	:	yes
Test substance	:	other TS: 711P
Method	:	Control Groups: The negative control article was the solvent (acetone) used in the assay. Ethylmethane sulfonate (EMS) was used as a positive control in the assays without S9 activaiton. Statistical Methods: The minimum criterion necessary to demonstrate mutagenesis was a mutation frequency that was at least 1.5 times the concurrent background frequency plus 10 x 10-6. The background frequency was defined as the average mutant frequency of the solvent negative controls.
Result	:	In the absence of activation, 0.75 to 6.0 ul/ml induced moderate to high toxicity (percent relative growths: 3.2% to 48.4%), but only a slight increase in mutation frequency at the highest doses. In the presence of a metabolic fraction, 0.125 to 1.5 ul/ml resulted in percent relative growths of 8.9% to 82.2% without increasing the incidence of mutations. Thus, the test compound was considered non-mutagenic in this assay.
Test condition	:	Mouse lymphoma cells were seeded into a series of tubes at 6 x 106 cells per tube. Dosed tubes were exposed for 4 hours to the test substance. An expression period of 48 hours was used; after the 48 hour expression time, 3 x 106 cells per plate were added to semi-solid selection medium containing 3 ug/ml trifluorothymidine (TFT) to score for mutant colonies and 200 cells per plate were added to cloning medium, without TFT, to evaluate viability. Mutant frequencies were calculated after 10-14 days incubation. Mutant and total colony count at each dose level were determined by triplicate plates.
Test substance	:	Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11). Data used as read-across to 111381-91-0 1,2-benzenedicarboxylic acid, nonyl undecyl ester.
Conclusion	:	Under conditions of this study the test substance was non-mutagenic in the mouse lymphoma assay with or without metabolic activation.
Reliability	:	(1) valid without restriction

12.11.2001 (1)

6. References

(1) E. Barber, M. Cifone, J. Rundell, R. Przygoda, B. Astill, E. Moran, A. Mulholland, E. Robinson and B. Schneider. (2000). Results in the L5178Y mouse lymphoma and the in vitro transformation of Balb 3T3 cell assays for eight phthalate esters. Journal of Applied Toxicology 20:69-80.

(2) European Union IUCLID database (ECB, 2000).

(3) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(4) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 117-84-0
CAS No.	:	117-84-0
EINECS Name	:	dioctyl phthalate
EINECS No.	:	204-214-7
TSCA Name	:	1,2-Benzenedicarboxylic acid, dioctyl ester
Molecular Formula	:	C24H38O4

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	09.11.2001
Revision date	:	
Date of last Update	:	09.11.2001
Number of Pages	:	14
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers:
68648-93-1
117-84-0
68515-40-2
68515-45-7
68515-43-5
84-77-5
3648-20-2
85507-79-5
111381-91-0
68515-47-9

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic

solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

Type : industrial
Category : Polymers industry
Remark : High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

2.1 MELTING POINT

Value : -25 - ° C
Decomposition : no at - ° C
Sublimation : no
Method :
Year :
GLP :
Test substance :
Remark : Literature review collecting data from a variety of sources.
Manufacturer's data or handbook value
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (11)

Value : 90 - ° C
Decomposition : no at - ° C
Sublimation : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Melting point calculation seems to give erroneously high results for the phthalate esters
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (3) invalid
10.10.2001 (8)

2.2 BOILING POINT

Value : 431 - ° C at 1013 hPa
Decomposition : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001 (8)

Value : 390 ° C at 1013 hPa
Decomposition : no
Method : other
Year : 2000
GLP :
Remark : Manufacturer's data or handbook value.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (4) not assignable
10.10.2001 (4)

2.4 VAPOUR PRESSURE

Value	:	.000000133 - hPa at 25° C
Decomposition	:	no
Method		other (measured)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

09.11.2001 (2)

Value	:	.000000457 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (8)

2.5 PARTITION COEFFICIENT

Log pow	:	7.73 - at 25° C
Method		other (measured)
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

15.12.2000 (3)

Log pow	:	8.06 - at 25° C
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Literature review collecting data from a variety of sources.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (11)

Log pow	:	8.54 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	

Test substance :
Method : Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (8)

2.6.1 WATER SOLUBILITY

Value : .00018 - mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other
Year : 2000
GLP :
Test substance :
Method : Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
09.11.2001 (8)

Value : .0005 - mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other
Year :
GLP :
Test substance :
Remark : Literature review collecting data from a variety of sources.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001 (11)

Value : .00249 - mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other
Year : 2000
GLP :
Test substance :
Remark : Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (1) valid without restriction
15.12.2000 (3)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.00000000002058 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (8)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	7.7 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

15.12.2000 (8)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.064
Water (level I)	:	.0003
Soil (level I)	:	97.7
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

Reliability : (2) valid with restrictions
10.10.2001

(7)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : other (calculation)
Year : 2000
Result : Soil - 97.7%
Air - 0.064%
Water - 0.00032%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001

(7)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	male
Number of animals	:	
Vehicle	:	no data
Value	:	= - 53700 mg/kg bw
Method	:	other
Year	:	1987
GLP	:	no data
Test substance	:	other TS
Test condition	:	Rangefinding study used to establish dose levels for subsequent 5-day study. Only LD50 value reported; no information on animal numbers, dose levels, etc. provided.
Test substance	:	1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate)
Conclusion	:	Under the conditions of this study, the test substance has a low order of acute oral toxicity in rats.
Reliability	:	(4) not assignable

09.11.2001 (9)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	male
Number of animals	:	
Vehicle	:	no data
Value	:	= - 13000 mg/kg bw
Method	:	other
Year	:	1989
GLP	:	no data
Test substance	:	other TS
Test condition	:	Rangefinding study used to establish dose levels for subsequent 5-day study. Only LD50 value reported; no information on animal numbers, dose levels, etc. provided.
Test substance	:	1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate)
Conclusion	:	Under the conditions of this study, the test substance has a low order of acute oral toxicity in mice.
Reliability	:	(4) not assignable

09.11.2001 (10)

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	Daily
Frequency of treatment	:	Daily for 13 weeks
Post obs. period	:	Not applicable
Doses	:	0, 5, 50, 500, or 5000 parts per million (0, 0.4, 3.8, 38.8, or 376.5 mg/kg/day).
Control group	:	yes
NOAEL	:	= - 38.8 mg/kg

Method	:	OECD Guide-line 408 "Subchronic Oral Toxicity - Rodent: 90-day Study"
Year	:	1997
GLP	:	no data
Test substance	:	other TS
Method	:	One-way analysis of variance and Duncan's multiple range test.
Remark	:	No clinical signs of toxicity, reductions in body weight or food consumption were observed throughout the study. At the highest dose, DNOP caused threefold (females) and 12-fold (males) increases in liver ethoxyresorufin-O-deethylase activity while DEHP did not. Both DEHP and DNOP at 5000 ppm caused mild histological changes in the thyroid consisting of reduced follicle size and colloid density, and the liver consisting of endothelial nuclear prominence, nuclear hyperchromicity and anisokaryosis. There was accentuation of zonation of the hepatic lobules and increased perivenous cytoplasmic vacuolation in DNOP-treated rats. DNOP did not induce any testicular changes or visible increases in the number of peroxisomes. Trace quantities (3-5 ppm) of DEHP and DNOP were detected in the liver, and 15-31 ppm were found in adipose tissue of the highest dose groups.
Test condition	:	Sprague-Dawley-rats were administered 0, 5, 50, 500, or 5,000 parts per million (ppm) di-n-octyl phthalate (DNOP) in their diet for 13 weeks. Similar control groups received either 4% corn oil or 5000 ppm of di(2-ethylhexyl) phthalate (DEHP). At termination, blood and tissue samples were obtained for selected analyses including specific liver enzymes, fat residue analysis, and peroxisome proliferation.
Test substance	:	1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate)
Conclusion	:	Limited signs of toxicity were observed in male and female rats administered DNOP in the diet for 13 weeks.
Reliability	:	(1) valid without restriction

10.10.2001 (1)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Bacterial
Concentration	:	5 dose levels up to 10 mg/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year	:	1985
GLP	:	no data
Test substance	:	other TS
Method	:	A mutagenic response was defined as a reproducible, dose-related increase in the number of histidine-independent colonies over the spontaneous incidence. There was no requirement for a specific magnitude of increase.
Test condition	:	Approximately 10E8 bacteria were mixed with 0.5 ml of either 0.1M sodium phosphate buffer or S-9 mix, and test substance. The reaction was carried out in triplicate. The mixture was incubated at 37°C for 48 hours, after which time histidine-revertant colonies were counted. The doses selected were separated by half-log intervals. The high dose was 10 mg/plate unless limited by solubility. Positive control chemicals were sodium azide, nitro-o-phenylenediamine, 9-aminoacridine and 2-aminoanthracene. Concurrent solvent and positive controls were included in all experiments. A toxicity pretest with TA 100 was conducted to determine the high dose level.
Test substance	:	1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate)
Conclusion	:	No mutagenic activity was observed at doses up to 10 mg/plate in Salmonella strains TA 98, TA 100, TA 1535 and TA 1537 with or without

metabolic activation.

Reliability : (1) valid without restriction
10.10.2001

(5)

5.8 TOXICITY TO REPRODUCTION

Type	:	Two generation study
Species	:	mouse
Sex	:	male/female
Strain	:	CD-1
Route of admin.	:	oral feed
Exposure period	:	Continuous throughout study (beginning 7 days prior to mating).
Frequency of treatment	:	Daily throughout premating, mating, gestation and lactation.
Premating exposure period		
Male	:	7 days
Female	:	7 days
Duration of test	:	2 generations
Doses	:	0.0, 1.25, 2.5, or 5.0% (0, 1.8, 3.6, and 7.5 g/kg/day)
Control group	:	yes
NOAEL Parental	:	= - 5 %
NOAEL F1 Offspr.	:	= - 5 %
NOAEL F2 Offspr.	:	= - 5 %
Method	:	other
Year	:	1987
GLP	:	no data
Test substance	:	other TS
Method	:	Cochran-Armitage (dose-related trends); Fisher's exact test (mating and fertility trends); Kruskal-Wallis test and Jonckheere's test (group means for sex ratio); Wilcoxon-Mann-Whitney U test (pairwise comparisons of treatment group means).
Remark	:	DNOP had no effect on any fertility or reproductive measure. There were no treatment-related changes in parental clinical signs, body weight gains, or food consumption. The only significant finding was increased liver weight in the high dose (5%) males and females and increased kidney weight in the high dose females.
Test condition	:	There were 40 animals/sex in the untreated control group. Males and females in the treatment groups (20 animals/sex) were exposed to the test substance beginning with a 7-day premating period and throughout a cohabitation period for approximately 14 weeks. Reproductive function was assessed during this cohabitation period for number of litters per pair, number of live pups, sex, live births, and pup weight. These litters were subsequently discarded. Following the 14-week cohabitation, the pairs were separated during which time any final litters were delivered and kept for assessment of the next generation fertility (F1). When the F1 litters were sexually mature, they were mated with animals from different litters within the same group. The F2 litters were examined for litter size, survival, sex and pup weight. The F1 animals were then sacrificed and necropsied. F0 parameters evaluated: clinical signs, mortality, body weight gain, consumption of food and water. F1 parameters evaluated: reproductive performance, litter size, survival, sex and pup weight F2 parameters evaluated: litter size, survival, sex and pup weight. Sperm examination: Epididymis from the right cauda was excised. The percentage of motile sperm, under 400 magnification was determined. Necropsies: In females, endpoints examined included organ weights and histology. In males, organ weights, histology, percentage of motile sperm, sperm concentration and percentage of abnormal sperm were assessed. Clinical observations were performed on blood and urine collected at the post-mortem examination.

Test substance	:	1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate)
Reliability	:	(1) valid without restriction

28.12.2000

(6)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	mouse
Sex	:	female
Strain	:	CD-1
Route of admin.	:	gavage
Exposure period	:	Gestation days 6-13
Frequency of treatment	:	Daily
Duration of test	:	7 Days
Doses	:	10 ml/kg/day (9780 mg/kg/day)
Control group	:	yes
NOAEL Maternalt.	:	= - 9780 mg/kg bw
NOAEL Teratogen	:	= - 9780 mg/kg bw
Method	:	other
Year	:	1987
GLP	:	no data
Test substance	:	other TS
Result	:	NOAEL: 9780 mg/kg/day (maternal and developmental). Maternal Effects: No mice died during the study. There were no clinical signs of toxicity or changes in food consumption or body weight. Embryo/fetal Effects: The only differences from the concurrent control group were a slightly reduced number of live births per litter (10.2 vs. 11.5) and reduced pup weight gain (0.6 g vs. 0.7g). However it was noted that the control values for these parameters were significantly higher than other control values in this study program, therefore the differences were not considered to be biologically significant.
Test condition	:	Fifty timed-pregnant female mice were dosed daily on gestation days 6-13 with the test substance. A single dose level of 10 ml/kg was used as the highest practical level due to lack of toxicity (LD10 could not be established). Litters were held until postpartum day 3 then discarded. The following data were recorded: maternal observations, survival, and weight gain from gestation day 6 to postpartum day 3; number of live births, number of viable litters, total litter weight, litter weight gain, and pup survival.
Test substance	:	1,2-benzenedicarboxylic acid, dioctyl ester (di-n-octyl phthalate)
Conclusion	:	No significant developmental effects were found at a single maximum dose level of 10 ml/kg/day (9780 mg/kg/day).
Reliability	:	(2) valid with restrictions

28.12.2000

(1)

6. References

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7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 119-06-2
CAS No.	:	119-06-2
EINECS Name	:	di(tridecyl) phthalate
EINECS No.	:	204-294-3
TSCA Name	:	1,2-Benzenedicarboxylic acid, ditridecyl ester
Molecular Formula	:	C34H58O4

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	03.10.2001

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	03.10.2001
Memo	:	ACC Phthalate Ester Panel HPV (read-across)
Printing date	:	12.11.2001
Revision date	:	
Date of last Update	:	04.10.2001
Number of Pages	:	11
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers:
68648-93-1
117-84-0
68515-40-2
68515-45-7
68515-43-5
84-77-5
3648-20-2
85507-79-5
111381-91-0
68515-47-9

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic

solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	5
Vehicle	:	other: corn oil
Value	:	> 2000 - mg/kg bw
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Test species/strain: Rat/Crj:CD(Sprague-Dawley) Test method: OECD Acute Oral Toxicity Test Route: Oral(Gavage) Doses: 0(vehicle), 2000 mg/kg Number of animals/group: Males, 5; females, 5
Remark	:	Study reports are in Japanese, however, the study summary and data tables are reported in English.
Result	:	No death occurred of either males or females in the treated groups. No effects were found on general condition, body weight changes or autopsy findings. LD50: Male, > 2000 mg/kg; female, > 2000 mg/kg
Test substance	:	ditridecyl phthalate (CAS No. 119-06-2). Purity: 93.7-100% (converted by ester value, 198-212).
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

04.10.2001 (2)

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Males, 42 days. Females, from 14 days prior to mating to day 3 of lactation
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	0(vehicle), 10, 50, 250 mg/kg/day
Control group	:	yes, concurrent vehicle
NOAEL	:	= 10 - mg/kg bw
LOAEL	:	= 50 - mg/kg bw
Method	:	OECD combined study TG422
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Test species/strain: Rat/Crj:CD(Sprague-Dawley) Test method: OECD Combined Repeat Dose and Reproductive/ Developmental Toxicity Screening Test Route: Oral(Gavage) Doses: 0(vehicle), 10, 50, 250 mg/kg/day

Number of animals/group: Males, 13; Females, 13

Vehicle: Corn oil

Administration period: Males, 42 days. Females, from 14 days prior to mating to day 3 of lactation

Terminal killing: Male, day 43. Females, day 4 of lactation

Remark : Study reports are in Japanese, however, the study summary and data tables are reported in English.

Result : No deaths were observed. Increased salivation was transiently observed in male animals of the 50 and 250 mg/kg groups after the day 10 of treatment until the autopsy. No adverse effects were detected on food consumption in males and females of any group, whereas suppression of body weight gain was observed in females of the 50 and 250 mg/kg groups. No adverse effects of ditridecyl phthalate were found on the general condition in females and on body weight gain in males.

Increase in liver weight was observed in males of the 250 mg/kg group and in females of the 50 and 250 mg/kg groups. On histopathological examination of liver, hypertrophy of the centrilobular hepatocytes was observed in males and females of the 50 and 250 mg/kg groups, and catalase positive granules in centrilobular hepatocytes were increased in males, as well. An increase in kidney weight was found in males of the 250 mg/kg group. On histopathological examination, eosinophilic bodies in renal tubular cells were increased in males of the 250 mg/kg group. In addition, basophilic tubules in the cortex which appeared to be regeneration foci resulting from necrosis of renal tubular epithelium were observed in this group. Hyperplasia of the pelvic epithelium and transitional cells of the urinary bladder was found in females of the 250 mg/kg group, while ditridecyl phthalate did not affect kidney weight in females. On urinary testing and hematological examination, no adverse effects of ditridecyl phthalate were noted. On blood chemical examination in males, ALP activity was found to be increased after the treatment of ditridecyl phthalate at 250 mg/kg.

No testicular toxicity was detected in any groups.

The no observed effect dose level(NOEL) for repeat dose toxicity is considered to be 10 mg/kg/day in males and females.

Test substance : ditridecyl phthalate (CAS No. 119-06-2).
Purity: 93.7-100 %(converted by ester value, 198-212)

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

04.10.2001 (1)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test

System of testing : S. typhimurium TA100, TA1535, TA98, TA1537,

Concentration : 156, 313, 625, 1250, 2500 and 5000 ug/plate.

Cycotoxic conc. : >5000 ug/plate

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"

Year :

GLP : yes

Test substance : as prescribed by 1.1 - 1.4

Method : Test species/strains: S. typhimurium TA100, TA1535, TA98, TA1537

Test method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan)and OECD Guidelines No. 471

Procedures: Pre-incubation method

Solvent: DMSO

Positive controls:-S9mix:2-(2-Furyl)-3-(5-nitro-2-furyl)acrylamide(TA100, TA98), Sodium azide(TA1535), 9-Aminoacridine hydrochloride(TA1537) +S9 mix; 2-Aminoanthracene(all strains)

S9:Rat liver, induced with phenobarbital and 5,6-benzoflavone

Plates/test: 3

Number of replicates: 2

Remark : Study reports are in Japanese, however, the study summary and data tables are reported in English.

Result : This chemical did not induce gene mutations in the S. typhimurium strains. No toxicity was observed up to a concentration of 5000 ug/plate, with or without metabolic activation.

Genetic effects:
S. typhimurium TA100, TA1535, TA98 and TA1537

	+	?	-
Without metabolic activation:	[ ]	[ ]	[*]
With metabolic activation:	[ ]	[ ]	[*]

Test substance : ditridecyl phthalate (CAS No. 119-06-2).
Purity: 99.82%

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

04.10.2001 (1)

Type : Escherichia coli reverse mutation assay

System of testing : E. coli WP2 uvrA

Concentration : 156, 313, 625, 1250, 2500 and 5000 ug/plate

Cycotoxic conc. : >5000 ug/plate

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 472 "Genetic Toxicology: Escherichia coli Reverse Mutation Assay"

Year :

GLP : yes

Test substance : as prescribed by 1.1 - 1.4

Method : Test species/strains: E. coli WP2 uvrA

Test method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan)and OECD Guidelines No. 472

Procedures: Pre-incubation method

Solvent: DMSO

Positive controls:
-S9 mix 2-(2-Furyl)-3-(5-nitro-2-furyl)acrylamide(WP2 uvrA)
+S9 mix; 2-Aminoanthracene(all strains)

S9:Rat liver, induced with phenobarbital and 5,6-benzoflavone

Plates/test: 3

Number of replicates: 2

Remark : Study reports are in Japanese, however, the study summary and data tables are reported in English.

Result : This chemical did not induce gene mutations in E. coli strains. No toxicity was observed up to a concentration of 5000 ug/plate, with or without metabolic activation.

Test substance : ditridecyl phthalate (CAS NO. 119-06-2).
Purity: 99.82%

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

04.10.2001 (1)

Type : Chromosomal aberration test

System of testing : Chinese hamster lung(CHL)cells

Concentration : 0, 1188, 2375, 4750 ug/mL

Cycotoxic conc. : >4750 ug/ml

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 473 "Genetic Toxicology: In vitro Mammalian Cytogenetic Test"

Year :

GLP : yes

Test substance : as prescribed by 1.1 - 1.4

Method : Type of cell used: Chinese hamster lung(CHL)cells

Test method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan)and OECD Guideline No. 473

Solvent: DMSO

Positive controls:
-S9 mix, Mitomycin C
+S9 mix, Cyclophosphamide

Doses:
-S9 mix(continuous exposure): 0, 1188, 2375, 4750 ug/mL
-S9 mix(short-term exposure): 0, 1188, 2375, 4750 ug/mL
+S9 mix(short-term exposure): 0, 1188, 2375, 4750 ug/mL

S9:Rat liver, induced with phenobarbital and 5,6-benzoflavone

Plates/test: 2

Remark : Study reports are in Japanese, however, the study summary and data tables are reported in English.

Result : Ditridecyl phthalate did not induce structural chromosomal aberrations and polyploidy in CHL cells, with or without an exogenous metabolic activation system.

Test substance : ditridecyl phthalate (CAS NO. 119-06-2)
purity: 99.82%

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

04.10.2001 (1)

5.8 TOXICITY TO REPRODUCTION

Type : One generation study

Species : rat

Sex : male/female

Strain : Sprague-Dawley

Route of admin.	:	gavage
Exposure period	:	Males, 42 days. Females, from 14 days prior to mating to day 3 of lactation.
Frequency of treatment	:	daily
Premating exposure period		
Male	:	14 days
Female	:	14 days
Duration of test	:	Male, 43 days. Female, from 14 days prior to mating to day 4 of lactation
Doses	:	0(vehicle), 10, 50, 250 mg/kg/day
Control group	:	yes, concurrent vehicle
NOAEL F1 Offspr.	:	= 250 - mg/kg bw
other:NOAEL parental (male)	:	= 250 - mg/kg bw
other:NOEL parental (female	:	= 50 - mg/kg bw
Method	:	OECD combined repeated dose and reproductive/developmental toxicity screening test
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Test species/strain: Rat/Crj:CD(Sprague-Dawley) Test method: OECD Combined Repeat Dose and Reproductive/ Developmental Toxicity Screening Test Route: Oral(Gavage) Doses: 0(vehicle), 10, 50, 250 mg/kg/day Number of animals/group : Males, 13; Females, 13 Vehicle: Corn oil Administration period: Males, 42 days. Females, from 14 days prior to mating to day 3 of lactation. Terminal killing: Male, day 43. Females, day 4 of lactation.
Remark	:	Study reports are in Japanese, however, the study summary and data tables are reported in English.
Result	:	No adverse effects were observed on copulation, fertility, maintenance of pregnancy, and delivery in any groups. A statistically significant decrease in live birth index on PND 0, possibly due to poor lactation, was observed in the 250 mg/kg group (87.7 in high dose vs 99.6 in controls). Viability of neonates on PND 4 was slightly decreased (not statistically significant) in the 250 mg/kg group (89.9 in the high dose vs. 96.8 in controls). However, there were no adverse effects of ditridecyl phthalate on sex ratio, body weight changes, and morphological appearance of pups. NOELs for reproductive and developmental toxicity are considered to be 250 mg/kg/day in males, 50 mg/kg/day in females, and 250 mg/kg/day in pups, respectively.
Test substance	:	ditridecyl phthalate (CAS No. 119-06-2). Purity: 93.7-100 %(converted by ester value, 198-212)
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

04.10.2001 (1)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Males, 42 days. Females, from 14 days prior to mating to day 3 of lactation.
Frequency of treatment	:	daily
Duration of test	:	Male, 43 days. Female, from 14 days prior to mating to day 4 of lactation
Doses	:	0(vehicle), 10, 50, 250 mg/kg/day
Control group	:	yes, concurrent vehicle
NOAEL Maternalt.	:	= -
NOAEL Teratogen	:	= 250 - mg/kg bw
other:NOEL maternal tox	:	= 10 - mg/kg bw
Method	:	other: OECD combined study TG422
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Test species/strain: Rat/Crj:CD(Sprague-Dawley)
Remark	:	tudy reports are in Japanese, however, the study summary and data tables are reported in English.
Result	:	There were no adverse effects of ditridecyl phthalate on sex ratio, body weight changes, and morphological appearance of pups. The NOAEL for developmental effects in pups was 250 mg/kg/day. Maternal effects included mild suppression of body weight gain (<10% decrease) and increased liver:body weight ratios in females of the 50 and 250 mg/kg groups. Other than slight liver hypertrophy, there were no adverse histopathologic findings in tissues of female rats. In addition, no adverse effects were observed on copulation, fertility, maintenance of pregnancy, and delivery in any groups. The NOEL for maternal effects was 10 mg/kg/day.
Test substance	:	ditridecyl phthalate (CAS No. 119-06-2) Purity: 93.7-100 %(converted by ester value, 198-212)
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

04.10.2001 (1)

6. References

(1) Japan Ministry of Health & Welfare (unpublished). Toxicity Testing Reports of Environmental Chemicals, Ditridecyl phthalate (CAS No. 119-06-2. hppt://wwwdb.mhlw.go.jp/ginc/cgi-bin/db1_search.pl?CAS=119-06-2.

(2) Japan Ministry of Health and Welfare (unpublished). Toxicity testing reports of environmental chemicals, Ditridecyl phthalate (CAS No. 119-06-2). hppt://wwwdb.mhlw.go.jp/ginc/cgi-bin/db1_search.pl?CAS=119-06-2.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 3648-20-2
CAS No.	:	3648-20-2
EINECS Name	:	diundecyl phthalate
EINECS No.	:	222-884-9
TSCA Name	:	1,2-Benzenedicarboxylic acid, diundecyl ester
Molecular Formula	:	C30H50O4

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - high MW phthalates
Printing date	:	12.11.2001
Revision date	:	
Date of last Update	:	12.11.2001
Number of Pages	:	17
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

01.11.2000

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment	This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers: 68648-93-1 117-84-0 68515-40-2 68515-45-7 68515-43-5 84-77-5 3648-20-2 85507-79-5 111381-91-0 68515-47-9
Remark	The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

2.1 MELTING POINT

Value : -9 - ° C
Decomposition : no at - ° C
Sublimation : no
Method :
Year :
GLP :
Test substance :
Remark : Literature review collecting data from a variety of sources. Manufacturer's data or handbook value
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
19.12.2000 (11)

Value : 156 - ° C
Decomposition : no at - ° C
Sublimation : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Melting point calculation seems to give erroneously high results for the phthalate esters
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (3) invalid
10.10.2001 (10)

2.2 BOILING POINT

Value : 501 - ° C at 1013 hPa
Decomposition : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Reliability : (2) valid with restrictions
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
10.10.2001 (10)

Value : 270 ° C at 1013 hPa
Decomposition : no
Method : other
Year : 2000
GLP :
Remark : Manufacturer's data or handbook value.
Reliability : (4) not assignable
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
10.10.2001 (6)

2.4 VAPOUR PRESSURE

Value	:	.00000000163 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (10)

Value	:	.00000000497 - hPa at 25° C
Decomposition	:	no
Method		other (measured)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

19.12.2000 (5)

2.5 PARTITION COEFFICIENT

Log pow	:	10.33 - at 25° C
Method		other (measured)
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

19.12.2000 (5)

Log pow	:	11.49 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

19.12.2000 (10)

2.6.1 WATER SOLUBILITY

Value	:	.00016 - other: ug/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (10)

Value	:	.00441 - other: ug/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

19.12.2000 (5)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.0000000000291 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

19.12.2000 (10)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	7.7 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

19.12.2000 (10)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	0
Water (level I)	:	0
Soil (level I)	:	97.8
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000

Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001 (9)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 2000
Result : Soil - 97.8%
Air - 0.0000346%
Water - 0.000000357%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
19.12.2000 (9)

3.5 BIODEGRADATION

Type : aerobic
Inoculum : domestic sewage
Concentration : 20mg/l related to Test substance
related to
Contact time : 28 day
Degradation : = 76 - % after
Result : readily biodegradable
Deg. Product :
Method : other
Year : 1983
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Method : Method/Guideline-USEPA 1982, CO2 Evolution, Shake Flask (modified Gledhill).
Inoculum-Domestic sewage, soil, and mineral medium.
Kinetics-Not Reported
Degradation Products-Not Reported
Analytical Monitoring-Yes
Result : Primary degradation is expressed as the loss of initial test substance. Ultimate biodegradation is expressed as the percentage of ThCO2 in each flask.

>99% primary biodegradation, 76.0% (sd 2.0) ultimate biodegradation.
Test condition : Inoculum was aged for 2 weeks prior to test initiation. The test chemical was added to flasks containing medium and inoculum. The flask were incubated and shaken in the dark for 28 days. Three replicates for CO2 evaluation and 4 replicates for primary degradation were tested. The CO2 production was captured in barium hydroxide solution. Primary biodegradation was determined at the beginning, middle and end by GC FID of entire contents of one replicate. A glucose and blank were also tested..

2L Erlenmeyer flasks were used as test vessels. The pH at initiation was 7.0 to 7.2. Test flasks were shaken at a rate of 120rpm at 22 +/- 2 Deg C.

Nominal test concentration = 20mg/L for test substance and glucose.
Test substance : Diundecyl Phthalate (CAS# 3648-20-2)

(1,2,-benzenedicarboxylic acid, diundecyl ester)
Synonym: DUP

Conclusion : The substance is readily biodegradable using mixed populations of microorganisms,

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

28.11.2000 (12)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	m >= 1.4 -
Method	:	other
Year	:	1982
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians. Statistical methods-Moving average angle, Probit or Bionomial
Result	:	No mortality was observed. Mean measured values used in calculation of LC50. Analytical samples taken at time zero and on a composite of replicates at termination. Measured values remained consistent during the exposure period. Undissolved test substance was observed on the surface of all test solutions on Day 0 and for the duration of exposure. Fish mean Total length=39mm, mean wet weight=0.5g
Test condition	:	Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15L of solution. The diluter maintained a water turnover rate of 5-8 tank volumes per day. Two replicates of ten organisms were tested per treatment. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection. Test temperature=11 +/- 1 Deg C., The pH range was 7.1 to 7.5. The mean Dissolved Oxygen ranged from 9.8 to 10.0 mg/L. Fish were obtained from a Maryland supplier. Nominal test concentrations: Control, 0.12, 0.25, 0.50, 1.0, and 2.0 mg/L. Mean measured test concentrations: <0.0091, 0.11, 0.20, 0.35, 0.88, and 1.4mg/L.
Test substance	:	Diundecyl Phthalate (CAS# 3648-20-2) (1,2,-benzenedicarboxylic acid, diundecyl ester) Synonym: DUP
Conclusion	:	Test substance is non-toxic to fish at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document.1
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

28.11.2000 (3)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)

Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	m > .02 -
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975 Statistical methods-Moving average angle, Probit or Bionomial
Result	:	Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined slightly during study exposure. More than 50% of the test organisms were trapped on the surface or air bubbles in the three highest concentrations during the study. A repeat test was performed at a loading of 10mg/L (measured values of 0.032 mg/L Day 0 and 0.007 mg/L Day 2). No mortality was observed at this highest water soluble concentration. LC50 value of >0.022 was recalculated to >0.02 as per USEPA current procedures using mean of measured initiation and termination samples 1.
Test condition	:	Test treatments were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 2 minutes. Dilutions of the stock were prepared for each treatment level. The stock solution was prepared at the highest treatment concentration. Three replicates of five organisms were tested per treatment. Test vessels were 250ml beakers with 200ml of test solution. Analytical method was Gas Liquid Chromatography (GLC). Test temperature=22 +/- 2 Deg C., The pH was 8.2 at initiation and was from 8.3 at Day 2. Dissolved Oxygen ranged from 7.6 to 7.9 at initiation and was 7.6 at Day 2. Daphnia were <24 hours old and obtained from in-house stock. Nominal test concentrations: control, 0.032, 0.055, 0.090, 0.15, and 0.25mg/L. Measured test concentrations <0.0087, 0.022, 0.044, 0.058, 0.10, 0.16/0.13mg/L (Day 0) Measured test concentrations <0.0087, <0.0087, <0.0087, 0.016, 0.028, and 0.044 mg/L (Day 2)
Test substance	:	Diundecyl Phthalate (CAS# 3648-20-2) (1,2,-benzenedicarboxylic acid, diundecyl ester) Synonym: DUP
Conclusion	:	Test substance is non-toxic to Daphnid at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document 1.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

28.11.2000 (2)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	
Exposure period	:	8 day
Unit	:	
Analytical monitoring	:	yes
EC50	:	m > 2.1 -
Method	:	other

Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-EPA 600/9-78-018, Printz Algal Assay Bottle Test, 1978. Test type-Static Acute Analytical Monitoring-Yes Statistical methods-Moving average angle, Probit or Bionomial
Result	:	In-vivo chlorophyll a, measured daily until less than 5% change. Both cell numbers and in-vivo chlorophyll a, measured at termination. Analytical samples taken at time zero and on a composite of replicates at termination. EC50 = >3.3 ppm based upon Day 0 measured values only. Value recalculated as >2.1 ppm as per USEPA current practices using mean of measured initiation and termination samples 1.
Test condition	:	Algal Growth Medium was used as the control and diluent. 10uL of test substance was added to 1.0L of sterile water to form a saturated phthalate solution. This solution was sonicated for 1 minute and allowed to settle for 4 hours. After settling, the water soluble fraction (WSF) was removed for testing. Initial algal concentration was 2.0x104 cells/ml. Only one treatment level was evaluated (100%WSF). Based upon earlier phthalate testing, toxicity was not expected. Lighting =4,700 lux, test temperature=22+/-2 Deg C. The pH range was 7.5 at initiation and 8.3 at Day 8. Algal culture stock obtained from Univ. of Texas at Austin. Nominal test concentrations: 100% WSF (10ul/L stock). Measured test concentrations = 3.3 ppm on Day 0, Measured test concentration = 0.85 ppm on Day 8
Test substance	:	Diundecyl Phthalate (CAS# 3648-20-2) (1,2,-benzenedicarboxylic acid, diundecyl ester) Synonym: DUP
Conclusion	:	Test substance is not toxic to algae at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document 1.
Reliability	:	(2) valid with restrictions Control chlorophyll or cell counts not reported.
Flag	:	Critical study for SIDS endpoint

28.11.2000

(4)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type	:	LD50
Species	:	mouse
Strain	:	ICR
Sex	:	male
Number of animals	:	10
Vehicle	:	other: none
Route of admin.	:	i.p.
Exposure time	:	
Value	:	> 100 - other: g/kg
Method	:	Other
Year	:	1975
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	No mortality at highest practical dose (100 g/kg).
Test condition	:	Groups of 10 male ICR mice were were administered the undiluted compound by intraperitoneal injection and observed for 7 days. The LD50, 95% confidence limits and slope were calculated the 7-day mortality data by Cornfeld and Mantel's (1950) modification of Karber's method.
Test substance	:	1,2-benzenedicarboxylic acid, diundecyl ester (diundecyl phthalate) CAS # 3648-20-2
Conclusion	:	The test substance produced no signs of toxicity at a dose level of 100g/kg (i.p).
Reliability	:	(2) valid with restrictions 2 - Reliable with restrictions. Limited experimental detail presented; only one sex tested.

01.11.2000 (13)

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	21 days
Frequency of treatment	:	Continuous
Post obs. period	:	None
Doses	:	0, 0.3, 1.2, 2.5% (~0, 282, 1145, and 2305 mg/kg/day)
Control group	:	yes, concurrent no treatment
NOAEL	:	= 282 - mg/kg bw
Method	:	other
Year	:	1985
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Statistical methods: not available
Result	:	NOAEL = 0.3% (approximately 282 mg/kg/day), based on decreased body weight gains and increased liver weights. Statistically significant decreases in body weight gain were observed at the mid and high dose for males and females. Slight changes in food consumption for both sexes were also observed; however, these changes were not statistically significant. At the mid and high dose, liver, and kidney weights were increased. In addition, increases were seen in liver enzymes and palmitoyl-CoA oxidation (an indicator of peroxisome proliferation Mid- and high-dose males also had increased relative testes weight, but no lesions were observed

histopathologically.

Test condition : Rats (n=5/sex/dose) were randomly assigned to the treatment groups. Following the acclimation period, the test or control diets were given to the rats for 21 days. The females received the test diets one day later than the males to allow the male and female necropsies to be conducted on consecutive days.

Test substance : 1,2-benzenedicarboxylic acid, diundecyl ester (diundecyl phthalate) CAS # 3648-20-2

Conclusion : The test substance was "mildly hepatotoxic" at levels of 1.2% and 2.5% in the diet of male rats.

Reliability : (2) valid with restrictions
2 - Reliable with restrictions. Limited hematological and serum chemistry endpoints evaluated.

Flag : Critical study for SIDS endpoint
01.11.2000

(1)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium /TA98; TA100; TA1535; TA1537
Concentration : 5 dose levels up to 10 mg/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year : 1985
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Method : A mutagenic response was defined as a reproducible, dose-related increase in the number of histidine-independent colonies over the spontaneous incidence. There was no requirement for a specific magnitude of increase.

Test condition : Approximately 108 bacteria were mixed with 0.5 ml of either 0.1M sodium phosphate buffer or S-9 mix, and test substance. The reaction was carried out in triplicate. The mixture was incubated at 37°C for 48 hours, after which time histidine-revertant colonies were counted. The doses selected were separated by half-log intervals. The high dose was 10 mg/plate unless limited by solubility. Positive control chemicals were sodium azide, nitro-o-phenylenediamine, 9-aminoacridine and 2-aminoanthracene. Concurrent solvent and positive controls were included in all experiments. A toxicity pretest was conducted to determine the high dose level. This study was conducted with TA 100 in the presence and absence of S-9.

Test substance : 1,2-benzenedicarboxylic acid, diundecyl ester (diundecyl phthalate) CAS # 3648-20-2

Conclusion : No mutagenic activity was observed at doses up to 10 mg/plate in Salmonella strains TA 98, TA 100, TA 1535 and TA 1537 with or without metabolic activation.

Reliability : (1) valid without restriction
1 - Valid without restrictions. NTP-sponsored study.

Flag : Critical study for SIDS endpoint
01.11.2000

(8)

Type : Mouse lymphoma assay
System of testing : Mouse lymphoma cells/L5178Y.
Concentration : 1 to 10 ul/ml
Cycotoxic conc. : 10 ul/ml
Metabolic activation : with and without
Result : negative

Method	:	OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year	:	2000
GLP	:	yes
Test substance	:	other TS: 711P
Method	:	Metabolic Activation: With and without Arochlor-induced rat liver S9 mixture. Control Groups: The negative control article was the solvent (acetone) used in the assay. Ethylmethane sulfonate (EMS) was used as a positive control in the assays without S9 activation. 3-methylcholanthrene which requires metabolic activation, was used as a positive control for assays with S9. Statistical Methods: The minimum criterion necessary to demonstrate mutagenesis was a mutation frequency that was at least 1.5 times the concurrent background frequency plus 10 x 10-6. The background frequency was defined as the average mutant frequency of the solvent negative controls.
Result	:	Cytotoxicity ranged from 3.5 - 21 % at the high dose levels. In the absence of activation, 2 to 10 ul/ml induced moderate to high toxicity (percent relative growths: 18.8% to 70.7%), but no increase in mutation frequency. In the presence of a metabolic fraction, 1 to 8 ul/ml was toxic (percent relative growths: 3.5% to 62.7%), without increasing the incidence of mutations. Thus, the test compound was considered non-mutagenic with activation in this assay.
Test condition	:	Mouse lymphoma cells were seeded into a series of tubes at 6 x 106 cells per tube. Dosed tubes were exposed for 4 hours to the test substance. An expression period of 48 hours was used; after the 48 hour expression time, 3 x 106 cells per plate were added to semi-solid selection medium containing 3 ug/ml triflourothymidine (TFT) to score for mutant colonies and 200 cells per plate were added to cloning medium, without TFT, to evaluate viability. Mutant frequencies were calculated after 10-14 days incubation. Mutant and total colony counts at each dose level were determined by triplicate plates.
Test substance	:	Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11). Data used as read-across to 3648-20-2 1,2-benzenedicarboxylic acid, diundecyl ester (diundecyl phthalate)
Conclusion	:	Under conditions of this study diundecyl phthalate was non-mutagenic in the mouse lymphoma assay with or without metabolic activation.
Reliability	:	(1) valid without restriction 1 - Reliable without restrictions.
Flag	:	Critical study for SIDS endpoint

12.11.2001 (7)

6. References

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1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(3) CMA Study, Acute Toxicity of Fourteen Esters to Rainbow Trout Salmo gairdneri Under Flow-Through Conditions. EG&G Bionomics, Inc. 1983. Report # BW-83-3-1373, Performed Jul 1982 to Jan 1983.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

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1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(5) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, Chemosphere 41:1389-1399.

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(8) E. Zeiger, S. Haworth, K. Mortelmans, and W. Speck (1985). Mutagenicity Testing of Di(2-ethylhexyl) phthalate and Related Chemicals in Salmonella. Environmental Mutagenesis 7: 213-232.

(9) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(10) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(11) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997), the Environmental Fate of Phthalate Esters: A literature Review, Chemosphere 35:667-749.

(12) Sugatt, R.H. et al, 1983 Shake Flask Biodegradation of 14 Commercial Phthalate Esters. Syracuse Research Corporation, Syracuse, NY. SRC# L1543-05. Performed for CMA.

(13) W. Lawrence, M. Malik, J. Turner, A. Singh and J. Autian. (1975). A toxicological investigation of some acute, short-term, and chronic effects of administering di-2-ethylhexyl phthalate (DEHP) and other phthalate esters. Environmental Research 9:1-11.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 68515-40-2
CAS No.	:	68515-40-2
TSCA Name	:	1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Synonym	:	Phthalic acid, benzyl alkyl(C7-C8) ester

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	09.11.2001
Revision date	:	
Date of last Update	:	09.11.2001
Number of Pages	:	14
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers:
68648-93-1
117-84-0
68515-40-2
68515-45-7
68515-43-5
84-77-5
3648-20-2
85507-79-5
111381-91-0
68515-47-9

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic

solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

2.1 MELTING POINT

Value	:	-37 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	
Remark	:	Literature review collecting data from a variety of sources. Manufacturer's data or handbook value
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (9)

Value	:	90 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation Melting point calculation seems to give erroneously high results for the phthalate esters
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(3) invalid

10.10.2001 (5)

2.2 BOILING POINT

Value	:	427 - ° C at 1013 hPa
Method	:	Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (5)

2.4 VAPOUR PRESSURE

Value	:	.000000579 - hPa at 25° C
Decomposition	:	
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

Reliability : (2) valid with restrictions
10.10.2001 (5)

2.5 PARTITION COEFFICIENT

Log pow : 6.74 - at 25° C
Method other (calculated)
Year : 2000
GLP :
Test substance :
Method : Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (5)

2.6.1 WATER SOLUBILITY

Value : .00847 - mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other
Year : 2000
GLP :
Test substance :
Method : Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001 (5)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.00000000000703 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (5)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	1.4 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (5)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.01
Water (level I)	:	.02
Soil (level I)	:	97.7
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

Reliability : (2) valid with restrictions
15.12.2000 (4)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 2000
Result : Soil - 97.7%
Air - 0.010%
Water - 0.020%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (4)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : no
LC50 : m > 1000 -
Method : other
Year : 1980
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Method : Method/Guideline-EPA-600/3-75-009, Methods for Acute Toxicity tests with Fish, Macroinvertebrates and Amphibians. 1975
Statistical methods-NA
Result : No mortality was observed.
No test substance insolubility was noted in report.

Fish mean total length=32.7 mm, mean wet weight=0.47g, Organism loading was not calculated.

Nominal test concentrations:

Loading Level (mg/L)	Mortality (96h)
Control	0
100	0
180	0
320	0
560	0
1000	0

Value-LC50=> 1000ppm.
Test condition : The test treatments were prepared by individually mixing the appropriate amount of test substance with 10ml of acetone and adding it directly to the test chambers. The control also received 10ml of solvent. One replicate was prepared for each test treatment and control. The test was performed in 5-gallon glass vessels containing 15L of dilution water. The dilution water was filter well water. Each treatment vessel contained 10 fish.

Test temperature=12 +/- 1 Deg C., The pH range was 7.5 to 7.9. The Dissolved Oxygen ranged from 8.0 to 8.9mg/L. Fish were obtained from Fender's Fish Hatchery in Baltic, Ohio.

Nominal test concentrations:Loading Level (mg/L)
Control, 100, 180, 320, 560, 1000
Test substance : Benzyl, C7-9 branched and linear phthalate (CAS# 68515-40-2)
Conclusion : Test substance is non-toxic to fish at or below its water solubility level.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
29.11.2000 (2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)

Unit	:	mg/l
Analytical monitoring	:	no
LC50	:	c 4.5 -
Method	:	other
Year	:	1979
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975 Statistical methods-Moving average angle, Probit or Bionomial
Result	:	Test organisms in the 1.0 and 1.8 mg/L loading levels were observed "clumped" together at 48 hours.

Nominal test concentrations:

Loading Level (mg/L)	Mortality (48 h)
Control	0
Solvent Control	0
1.0	0
1.8	2
3.2	6
5.6	13
10.0	20

Units-LC50
Value-4.5 mg/L (CI of 3.5 to 5.9) based upon nominal loading levels.

Test condition : Test treatments were prepared by adding the test substance with acetone directly to the test treatments. Two replicates of ten organisms were tested per treatment except the controls, which were tested with one replicate. Test vessels were 250ml beakers with 200ml of test solution. The dilution water was well water.

Test temperature=20 +/- 1 Deg C.,
The pH ranged from 7.8 to 8.1 during the study. Dissolved Oxygen ranged from 8.9 to 9.3 mg/L. Dilution water hardness was 240mg/L and Alkalinity was 360mg/L. Daphnia were <24 hours old and obtained from in-house stock. Lighting was 16 hours light and 8 hours dark (no intensity reported).

Nominal test concentrations:Loading Level (mg/L)
Control, Solvent Control, 1.0, 1.8, 3.2, 5.6, 10.0

Test substance	:	Benzyl, C7-9 branched and linear phthalate (CAS# 68515-40-2)
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

29.11.2000 (1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC50	:	m = 674 -
Method	:	other
Year	:	1979
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-EPA, Algal Assay Procedure: Bottle Test, 1971. Test type-Static Acute

Statistical methods-NA

Result : In-vivo chlorophyll, was measured daily. Both cell numbers and in-vivo chlorophyll, measured at termination.
Chlorophyll measured using a Turner filter flourometer. Cell counts performed via a hemacytometer.

% Difference at 96h

Loading Level (mg/L)	Chlorophyll	Cell #
Control	---	---
56	-8	-6
100	-12	-6
180	-18	-19
320	-20	-24
560	-55	-63
1000	-61	-69

Units-ppm
Value-EC50=674 ppm, based upon in-vivo chlorophyll measurements.
EC50=521ppm, based upon cell numbers.

Test condition : The appropriate amount of test substance was added directly to algal growth medium (control and diluent) to form individual treatment concentrations. The test was performed in 125ml flasks. The initial algal concentration was 3.0x104 cells per ml.

Lighting =4,000lux, Test temperature=24+/-1 Deg C. The pH range was 7.2 to 7.6. Algal culture stock obtained from USEPA Environmental Research Laboratory, Corvallis, Oregon.

Nominal test concentrations: control, 56, 100, 180, 320, 560, and 1,000 mg/L.

Test substance : Benzyl, C7-9 Branched and Linear Phthalate (CAS# 68515-40-2)

Reliability : (2) valid with restrictions
No final cell counts reported.
Limited details on test treatment preparation in report.
"Globules" of test material were observed in all test flasks during the study.

Flag : Critical study for SIDS endpoint

09.11.2001

(3)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	5
Vehicle	:	other: Undiluted test material administered
Value	:	> - 15800 mg/kg bw
Method	:	other
Year	:	1976
GLP	:	no
Test substance	:	
Test condition	:	The undiluted test material was fed by stomach tube to a single group of rats at a dose level of 15800 mg/kg. 5 rats (3 male, 2 female) were used. The rats were observed for toxic signs and sacrificed after 14 days.
Test substance	:	1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters. CAS # 68515-40-2
Conclusion	:	The compound was found to be non-lethal by oral ingestion in male and female rats at a dose of 15800 mg/kg.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

10.10.2001

(6)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	3
Vehicle	:	other: Undiluted test material administered
Value	:	> - 7940 mg/kg bw
Method	:	other
Year	:	1976
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	No animals died at either dose level. Toxic signs reported as reduced appetite and activity for 1 to 3 days. All rabbits appeared normal at necropsy.
Test condition	:	The undiluted compound was applied at doses of 5010 and 7940 mg/kg to the closely clipped, intact skin of rabbits. The treated areas were covered with plastic strips and animals held in wooden stocks for up to 24 hours, after which they were held in individual cages. The rabbits were observed for toxic signs daily for 14 days. Surviving animals were sacrificed after 14 days and observed for internal macroscopic abnormalities.
Test substance	:	1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters. CAS # 68515-40-2
Conclusion	:	The test substance was considered practically non-toxic by dermal exposure in male and female rabbits.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

10.10.2001

(7)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Bacterial
Concentration	:	0.01, 0.04, 0.2, 1.0, 3.0, and 10.0 ul/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year	:	1982
GLP	:	yes
Test substance	:	
Method	:	Statistical analysis was performed on the results after transforming values to log10. Analysis included Bartlett's test for homogeneity of variance and comparison to controls with a t-test. Dose-response was evaluated with regression analysis and significance of the response evaluated by a t-test.
Remark	:	The substance was not mutagenic at doses < 10 mg/plate in Salmonella strains TA98, TA 100, TA 1535, TA 1537 and TA1538 in plate incorporation assays with or without metabolic activation. No microbial toxicity was observed in any of the five strains at 10 mg/plate with or without metabolic activation, although levels of 3 ug/plate and higher exceeded the solubility of the test material.
Test condition	:	Positive control chemicals were sodium nitrite, 9-aminoacridine, and 4-nitroquinoline-N-oxide (without S9); or benzo(a)pyrene, 2-acetylaminofluorene, and 2-aminoanthracene (with S9); the solvent control was DMSO. Concurrent solvent and positive controls were included in all experiments. A toxicity pretest with TA100 was conducted with and without microsomal activation to determine the highest dose level. The plate incorporation tests were conducted in all strains with and without activation.
Test substance	:	1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters. CAS # 68515-40-2
Conclusion	:	The test substance was not mutagenic in all strains tested.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

10.10.2001 (8)

6. References

(1) Analytical Bio Chemistry Laboratories, Inc (ABC), Static Acute Bioassay #23040-B, for Monsanto Chemical Company, St. Louis, MO. 1979.

(2) Analytical Bio Chemistry Laboratories, Inc (ABC), Static Acute Bioassay #25427, for Monsanto Chemical Company, St. Louis, MO. 1980.

(3) EG&G, Bionomics Marine Research Laboratory, Freshwater Alga Toxicity Test with Selenastrum capricornutum. Report # BP-79-2-20 for Monsanto Chemical Company, St. Louis, MO. 1979.

(4) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(5) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(6) Monsanto Company (1976). Acute oral toxicity with Santicizer 261. Unpublished report.

(7) Monsanto Company (1976). Minimum Lethal Dose by Skin Adsorption in Rabbits with Santicizer 261. Unpublished report.

(8) Monsanto Research Corporation (1982). Salmonella Mutagenicity Assay of Santicizer 261. Unpublished report.

(9) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997), the Environmental Fate of Phthalate Esters: A literature Review, Chemosphere 35:667-749.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 68515-41-3
CAS No.	:	68515-41-3
EINECS Name	:	1,2-Benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
EINECS No.	:	271-083-0

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	04.10.2001

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	04.10.2001
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	12.11.2001
Revision date	:	
Date of last Update	:	12.11.2001
Number of Pages	:	10
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers:
68648-93-1
117-84-0
68515-40-2
68515-45-7
68515-43-5
84-77-5
3648-20-2
85507-79-5
111381-91-0
68515-47-9

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic

solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	predominantly domestic sewage
Concentration	:	200mg/l related to Test substance related to
Contact time	:	
Degradation	:	> 99 - % after 28 day
Result	:	readily biodegradable
Kinetic of test substance	:	3 day = 2 - % 7 day = 21 - % 9 day = 27 - % 14 day = 40 - % 28 day = 53 - %
Deg. Product	:	
Method	:	other: EPA 560/6-82-003
Year	:	1982
GLP	:	no data
Test substance	:	other TS: unspecified DIOP
Source	:	Exxon Chemical Europe Inc. Bruxelles

05.01.1993

(9)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 22000 - mg/kg bw
Method	:	other: not specified
Year	:	1975
GLP	:	no data
Test substance	:	other TS: unspecified isomer
Source	:	Exxon Chemical Europe Inc. Bruxelles

21.12.1992 (3)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 26000 - mg/kg bw
Method	:	other: not specified
Year	:	1975
GLP	:	no data
Test substance	:	other TS: unspecified isomer
Source	:	Exxon Chemical Europe Inc. Bruxelles

21.12.1992 (2)

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male/female
Strain	:	other: not specified
Route of admin.	:	oral feed
Exposure period	:	4 weeks
Frequency of treatment	:	daily
Post obs. period	:	
Doses	:	not stated
Control group	:	yes
NOAEL	:	= 100 - mg/kg
Method	:	other: not specified
Year	:	1973
GLP	:	no data
Test substance	:	other TS: unspecified DIOP
Source	:	Exxon Chemical Europe Inc. Bruxelles

23.12.1992 (7)

Species	:	dog
Sex	:	male/female
Strain	:	other: not specified
Route of admin.	:	oral feed
Exposure period	:	14 weeks

Frequency of treatment	:	daily
Post obs. period	:	
Doses	:	not specified
Control group	:	yes
NOAEL	:	= 100 - mg/kg
Method	:	other: not specified
Year	:	1973
GLP	:	no data
Test substance	:	other TS: unspecified DIOP
Source	:	Exxon Chemical Europe Inc. Bruxelles

23.12.1992 (8)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella typhimurium strains TA 98, 100, 1535 and 1537.
Concentration	:	10 to 2000 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: unspecified DIOP
Source	:	Exxon Chemical Europe Inc. Bruxelles

05.01.1993 (6)

Type	:	other: Modified Ames fluctuation test
System of testing	:	modified Ames
Concentration	:	not stated
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	ambiguous
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: unspecified DIOP
Remark	:	A commercial grade of DIOP was weakly mutagenic to the bacterium Salmonella typhimurium in the presence, but not in the absence, of a liver metabolic activation system. The results were considered equivocal as no consistent dose related response was seen and the mutagenic activity only occurred within a narrow concentration range.
Source	:	Exxon Chemical Europe Inc. Bruxelles

23.12.1992 (1)

Type	:	other: cell transformation assay
System of testing	:	BALB/C-3T3 cells
Concentration	:	0.13, 1.25, 4.25, 12.70, or 42.35 ug/ml
Cycotoxic conc.	:	
Metabolic activation	:	no data
Result	:	negative
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: unspecified DIOP
Source	:	Exxon Chemical Europe Inc. Bruxelles

05.01.1993 (4)

5.8 TOXICITY TO REPRODUCTION

Type	:	Two generation study
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	Continuous throughout study
Frequency of treatment	:	Daily over two generations
Premating exposure period		
Male	:	10 weeks
Female	:	10 weeks
Duration of test	:	2 generation
Doses	:	0.0, 0.1, 0.5, or 1.0%.
Control group	:	yes
NOAEL Parental	:	= - 1 %
NOAEL F1 Offspr.	:	= - 1 %
other: systemic effects	:	= - .5 %
Method	:	EPA OPPTS 870.3800
Year	:	2000
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	Bisoflex L79P (di-(C7-C9 alkyl), is a phthalate ester based upon a linear alcohol, Linevol 79. Linevol 79 has alkyl chains with carbon distributions of >96% in the range C7 to C9 (typically 39 to 50% C7 , 17 to 28% C8 , and 27 to 39% C9). Linevol 79 has a minimum of 80% normality with predominant mono-2-methyl branching.
Method	:	Statistical Methods: Organ and body weight data assessed by Bartlett's test for homogeneity of variance; then pairwise comparisons by Behren's-Fisher test or Dunnett's test. Intergroup differences in macroscopic and microscopic pathology assessed by Fisher's exact test. Food consumption and litter data analyzed by ANOVA (parametric) or Kruskal-Wallis test (non-parametric) as appropriate.
Test condition	:	F0 males and females (28 animals/sex) were exposed to the test substance for 10 weeks prior to mating. One male and one female were paired for up to 3 weeks. F0 offspring were examined 24 hours after birth and number of pups, body weights, sex, and gross observations. Litters were culled to 4 male and 4 female pups and at PND 25 selected for the next (F1) generation. Parental (F0) males and females were necropsied, organs weighed and microscopically examined. Epididymal fluid was obtained for sperm analysis, uteri were examined for implantation sites. Livers from five males/group were analyzed for protein content and cyanide-insensitive palmitoyl CoA oxidase activity. Body weights and food consumption were recorded weekly throughout the study, and clinical observations recorded twice daily
Result	:	NOAEL - 1.0% in diet for reproductive endpoints; 0.5% for general toxicity.
Remark	:	The 1.0% males showed reduced body weights in both the F0 and F1 generations. There was no impairment of fertility, fecundity, or development in either generation, but pup body weights were slightly reduced in the 1.0% group over the weaning period. Ovary weights were decreased in the 1.0% group for both generations, although ovarian function as assessed by estrus cycle and mating behavior was not affected. Liver changes indicative of peroxisomal proliferation were noted in both generations and both sexes at the high dose (1%), characterized by increased liver weight in young rats, histopathological changes and decreased weights in mature rats, and an increase in palmitoyl CoA oxidase activity.

Conclusion	:	The test substance did not impair reproductive function in rats at any level tested. Signs of systemic toxicity were observed at 1.0%.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

12.11.2001

(10)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	GD 1 through GD 19
Frequency of treatment	:	daily
Duration of test	:	20 days
Doses	:	250, 500, or 1000 mg/kg
Control group	:	yes, concurrent vehicle
NOAEL Maternalt.	:	= 1000 mg/kg bw
NOAEL Teratogen	:	= 500 mg/kg bw
Method	:	other:EPA OPPTS 870.3700
Year	:	2001
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	Bisoflex L79P (di-(C7-C9 alkyl). Is a phthalate ester based upon a linear alcohol, Linevol 79. Linevol 79 has alkyl chains with carbon distributions of >96% in the range C7 to C9 (typically 39 to 50% C7 , 17 to 28% C8 , and 27 to 39% C9. Linevol 79 has a minimum of 80% normality with predominant mono-2-methyl branching.
Method	:	For Statistical Analysis: Homogeneity of variance was assessed using Barlett's test, and data were analyzed with parametric tests (analysis of variance followed by Williams' test) or nonparametric tests (kruskal-Wallis followed by Shirley's test) as appropriate. Data on fetal malformations and variations was analyzed using categorical data models.
Test condition	:	A total of 220 virgin female Sprague-Dawley rats were mated on a 1:1 basis with stock males from the same strain and source. The day that a positive indication of mating was observed (i.e. sperm-positive vaginal smear or at least three copulation plugs) was designated day 0 of gestation (GD 0).
Result	:	The NOAEL for maternal toxicity was 1000 mg/kg/day. The NOAEL for the developmental toxicity of D79P was 500 mg/kg/day, based on an increased incidence of skeletal variations at the high dose. The biological significance of skeletal variations is questionable.
Remark	:	There were no effects on the incidence of external or visceral abnormalities. An increased incidence of supernumerary lumbar ribs occurred at doses of 1000 mg/kg/day. However, this common skeletal variation is not an indicator of a teratogenic effect. There were no statistical significant differences in bodyweight, fertility, reproductive organs, litter size, placental weights or fetal survival between any treatment groups and the prospective control groups at any time during gestation. There were no remarkable macroscopic findings in the maternal animals at necropsy. Fetal, litter, and placental weights were all unaffected by treatment with D79P.
Conclusion	:	Under the conditions of this study the test substance did not induce any evidence of maternal toxicity, embryofetal lethality or teratogenicity.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

12.11.2001

(5)

6. References

(1) BIBRA (1989). Toxicity Profile for Diisooctyl Phthalate.

(2) BIBRA Toxicity Profile (1989) Diisooctyl Phthalate.

(3) BIBRA Toxicity Profile (1989). Diisooctyl Phthalate.

(4) Evaluation of Diisooctyl Phthalate in the In Vitro Transformation of BALB/C-3T3 Cells Assay, Final Report (1981). Litton Bionetics, Inc. EPA Document #878210226.

(5) Fulcher S.M., C.R. Willoughby, J.A. Heath, G.E. Veenstra and N Moore (2001). Developmental toxicity of di-(C7-C9 alkyl) phthalate and di-(C9-C11 alkyl) phthalate in the rat. Repro. Toxicol. 15: 95-102.

(6) Mutagenicity Evaluation of Diisooctyl Phthalate (USS Chemical). Goodyear Fiber and Polymer Products Research Division. Laboratory Report No. 81-4-7. EPA Document #878210226.

(7) Shibko, S. I. and Blumenthal, H. (1973). Toxicology of Phthalic Acid Esters Used in Food-Packaging Materials. Enrivon. Health Perspec., January 1973, p. 131-137.

(8) Shibko, S. I. and Blumenthal, H. (1973). Toxicology of Phthalic Acid Esters Used in Food-Packaging Materials. Environ. Health Perspect., January 1973, p. 131-137.

(9) Sugatt, R. H. et. al. (1984). Shake Flask Biodegradation of 14 Commercial Phthalate Esters. Appl. Environ. Micro. 47(4): 601-606.

(10) Willoughby, C.R., Fulcher, S.M., Creasy, D.M., Heath, J.A., Priston, R.A.J., and Moore, N.P. (2000). Two generation reproduction toxicity studies of di-(C7-C9 alkyl) phthalate and di-(C9-C11 alkyl) phthalate in the rat. Reproductive Toxicology 14: 427-450.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 68515-43-5
CAS No.	:	68515-43-5
EINECS Name	:	1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters
EINECS No.	:	271-085-1
TSCA Name	:	1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - high MW phthalates
Printing date	:	12.11.2001
Revision date	:	
Date of last Update	:	12.11.2001
Number of Pages	:	12
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers:
68648-93-1
117-84-0
68515-40-2
68515-45-7
68515-43-5
84-77-5
3648-20-2
85507-79-5
111381-91-0
68515-47-9

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to

their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

2.1 MELTING POINT

Value	:	-50 - ° C
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(4) not assignable
15.12.2000		(1)

Value	:	138 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation Melting point calculation by MPBPWIN ver. 1.04 using calculation methods of Joback and Gold and Ogle.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(3) invalid
10.10.2001		(4)

2.2 BOILING POINT

Value	:	466 ° C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Boiling point calculation by MPBPWIN ver 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions
10.10.2001		(4)

2.4 VAPOUR PRESSURE

Value	:	.0000000204 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

Reliability : (2) valid with restrictions
10.10.2001 (4)

2.5 PARTITION COEFFICIENT

Log pow : 10.39 - at 25° C
Method other (calculated)
Year : 2000
GLP :
Test substance :
Method : Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (4)

2.6.1 WATER SOLUBILITY

Value : .00209 - other: ug/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other
Year : 2000
GLP :
Test substance :
Method : Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001 (4)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.00000000002259 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

19.12.2000 (4)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	4.7 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (4)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.0004
Water (level I)	:	0
Soil (level I)	:	97.8
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000

Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (3)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 2000
Result : Soil - 97.8%
Air - 0.0004%
Water - 0.0000045%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
19.12.2000 (3)

5.8 TOXICITY TO REPRODUCTION

Type	:	Two generation study
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	Continuous throughout study
Frequency of treatment	:	Daily over two generations.
Premating exposure period		
Male	:	10 weeks
Female	:	10 weeks
Duration of test	:	2 generations
Doses	:	0.0, 0.1, 0.5, or 1.0%.
Control group	:	yes
NOAEL Parental	:	= 1 %
NOAEL F1 Offspr.	:	= 1 %
other: systemic effects	:	= 0.5 %
Method	:	EPA OPPTS 870.3800
Year	:	2000
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	Bisoflex L911P (di-(C9-C11 alkyl) phthalate, D911P; is a phthalate ester based upon a linear alcohol Linevol 911. Linevol 911 has alkyl chains with carbon distributions of >97% in the range C9 to C11 (typically 13 to 23% C9 , 37 to 47% C10 , and 33 to 43% C11). Linevol 911 has a minimum of 80% normality with predominant mono-2-methyl branching.
Method	:	Statistical Methods: Organ and body weight data assessed by Bartlett's test for homogeneity of variance; then pairwise comparisons by Behren's-Fisher test or Dunnett's test. Intergroup differences in macroscopic and microscopic pathology assessed by Fisher's exact test. Food consumption and litter data analyzed by ANOVA (parametric) or Kruskal-Wallis test (non-parametric) as appropriate.
Test condition	:	F0 males and females (28 animals/sex) were exposed to the test substance for 10 weeks prior to mating. One male and one female were paired for up to 3 weeks. F0 offspring were examined 24 hours after birth and number of pups, body weights, sex, and gross observations. Litters were culled to 4 male and 4 female pups and at PND 25 selected for the next (F1) generation. Parental (F0) males and females were necropsied, organs weighed and microscopically examined. Epididymal fluid was obtained for sperm analysis, uteri were examined for implantation sites. Livers from five males/group were analyzed for protein content and cyanide-insensitive palmitoyl CoA oxidase activity. Body weights and food consumption were recorded weekly throughout the study, and clinical observations recorded twice daily
Result	:	NOAEL - 1.0% in diet for reproductive function; 0.5% for general toxicity.
Remark	:	The 1.0% males showed reduced body weights in both the F0 and F1 generations. There was no impairment of fertility, fecundity, or development in either generation, but pup body weights were slightly reduced in the 1.0% group over the weaning period. Epididymal weights were decreased in the 1.0% group for both generations, although sperm concentration, motility, and morphology was not affected. Liver changes indicative of peroxisomal proliferation were noted in both generations and both sexes at the high dose (1%), characterized by increased liver weight in young rats, histopathological changes and decreased weights in mature rats, and an increase in palmitoyl CoA oxidase activity.
Conclusion	:	The test substance did not impair reproductive function in rats at any level

tested. Signs of systemic toxicity were observed at 1.0%.

Reliability : (1) valid without restriction
12.11.2001

(5)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	GD 1 through GD 19
Frequency of treatment	:	Daily
Duration of test	:	20 Days
Doses	:	250, 500, or 1000 mg/kg
Control group	:	yes, concurrent vehicle
NOAEL Maternalt.	:	= - 1000 mg/kg bw
NOAEL Teratogen	:	= - 250 mg/kg bw
Method	:	other:EPA OPPTS 870.3700
Year	:	2001
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	Bisoflex L911P (di-(C9-C11 alkyl) phthalate, D911P; is a phthalate ester based upon a linear alcohol Linevol 911. Linevol 911 has alkyl chains with carbon distributions of >97% in the range C9 to C11 (typically 13 to 23% C9 , 37 to 47% C10 , and 33 to 43% C11). Linevol 911 has a minimum of 80% normality with predominant mono-2-methyl branching.
Method	:	For Statistical Analysis: Homogeneity of variance was assessed using Barlett's test, and data were analyzed with parametric tests (analysis of variance followed by Williams' test) or nonparametric tests (kruskal-Wallis followed by Shirley's test) as appropriate. Data on fetal malformations and variations was analyzed using categorical data models.
Test condition	:	A total of 220 virgin female Sprague-Dawley rats were mated on a 1:1 basis with stock males from the same strain and source. The day that a positive indication of mating was observed (i.e. sperm-positive vaginal smear or at least three copulation plugs) was designated day 0 of gestation (GD 0).
Result	:	The NOAEL for maternal toxicity was 1000 mg/kg/day. The NOAEL value for the developmental toxicity of D911P was 250 mg/kg/day, based on minor skeletal and visceral variations. No malformations were observed at any dose level.
Remark	:	There were no effects on the incidence of external or visceral abnormalities. An increased incidence of dilated renal pelves was observed in the groups treated with 1000 mg/kg/day D911P, there was a significant trend with treatment (P< 0.01). An increased incidence of supernumerary lumbar ribs was observed at the mid (500 mg/kg/day) and high (1000 mg/kg/day) dose groups. However, these minor variations are commonly observed in rodents and are not considered to be an indicator of a teratogenic effect. There were no statistical significant differences in bodyweight, fertility, reproductive organs, litter size, placental weights or fetal survival between any treatment groups and the prospective control groups at any time during gestation. There were no remarkable macroscopic findings in the maternal animals at necropsy. Fetal, litter, and placental weights were all unaffected by treatment with D911P.
Conclusion	:	Under the conditions of this study the test substance did not induce any evidence of maternal toxicity, embryofetal lethality or teratogenicity.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
12.11.2001 (2)

6. References

(1) European Union IUCLID database, ECB 2000.

(2) Fulcher S.M., C.R. Willoughby, JA Heath, GE Veenstra and N Moore (2001). Developmental toxicity of di-(C7-C9 alkyl) phthalate and di-(C9-C11 alkyl) phthalate in the rat. Repro. Toxicol. 15: 95-102.

(3) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(4) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(5) Willoughby, C.R., Fulcher, S.M., Creasy, D.M., Heath, J.A., Priston, R.A.J., and Moore, N.P. (2000). Two generation reproduction toxicity studies of di-(C7-C9 alkyl) phthalate and di-(C9-C11 alkyl) phthalate in the rat. Reproductive Toxicology 14: 427-450.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 68515-45-7
CAS No.	:	68515-45-7
TSCA Name	:	1,2-benzenedicarboxylic acid, dinonyl ester, branched and linear
Generic name	:	dinonyl phthalate, branched and linear
Synonym	:	Phthalic acid, dialkyl(C9) ester

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - high MW phthalates
Printing date	:	12.11.2001
Revision date	:	
Date of last Update	:	12.11.2001
Number of Pages	:	11
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers:
68648-93-1
117-84-0
68515-40-2
68515-45-7
68515-43-5
84-77-5
3648-20-2
85507-79-5
111381-91-0
68515-47-9

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to

their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

2.1 MELTING POINT

Value : -48 - ° C
Decomposition : no at - ° C
Sublimation : no
Method :
Year :
GLP :
Test substance :
Remark : Literature review collecting data from a variety of sources.
Manufacturer's data or handbook value
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001 (6)

Value : 115 - ° C
Decomposition : no at - ° C
Sublimation : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Melting point calculation seems to give erroneously high results for the phthalate esters
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (3) invalid
10.10.2001 (5)

2.2 BOILING POINT

Value : 454 - ° C at 1013 hPa
Decomposition : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001 (5)

Value : >400 ° C at 1013 hPa
Decomposition : no
Method : other
Year : 2000
GLP :
Remark : Manufacturer's data or handbook value.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (4) not assignable
10.10.2001 (2)

2.4 VAPOUR PRESSURE

Value	:	.000000066 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (5)

Value	:	.0000000681 - hPa at 25° C
Decomposition	:	no
Method		other (measured)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

15.12.2000 (1)

2.5 PARTITION COEFFICIENT

Log pow	:	8.6 - at 25° C
Method		other (measured)
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

15.12.2000 (1)

Log pow	:	9.52 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (5)

15.12.2000

2.6.1 WATER SOLUBILITY

Value	:	.00002 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (5)

Value	:	.00031 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

15.12.2000 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.0000000000234 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (5)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	7.7 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (5)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.0011
Water (level I)	:	0
Soil (level I)	:	97.8
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000

Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000

(4)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 2000
Result : Soil - 97.8%
Air - 0.00107%
Water - 0.000033%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001

(4)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Mouse lymphoma assay
System of testing	:	Mammalian Cell
Concentration	:	0.125 to 6 ul/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year	:	2000
GLP	:	yes
Test substance	:	other TS: 711P
Method	:	Control Groups: The negative control article was the solvent (acetone) used in the assay. Ethylmethane sulfonate (EMS) was used as a positive control in the assays without S9 activation. 3-methylcholanthrene which requires metabolic activation, was used as a positive control for assays with S9. Statistical Medthods: The minimum criterion necessary to demonstrate mutagenesis was a mutation frequency that was at least 1.5 times the concurrent background frequency plus 10 x 10-6. The background frequency was defined as the average mutant frequency of the solvent negative controls.
Result	:	In the absence of activation, 0.75 to 6.0 ul/ml induced moderate to high toxicity (percent relative growths: 3.2% to 48.4%), but only a slight increase in mutation frequency at the highest doses. In the presence of a metabolic fraction, 0.125 to 1.5 ul/ml resulted in percent relative growths of 8.9% to 82.2% without increasing the incidence of mutations. Thus, the test compound was considered non-mutagenic in this assay.
Test condition	:	Mouse lymphoma cells were seeded into a series of tubes at 6 x 106 cells per tube. Dosed tubes were exposed for 4 hours to the test substance. An expression period of 48 hours was used; after the 48 hour expression time, 3 x 106 cells per plate were added to semi-solid selection medium containing 3 ug/ml trifluorothymidine (TFT) to score for mutant colonies and 200 cells per plate were added to cloning medium, without TFT, to evaluate viability. Mutant frequencies were calculated after 10-14 days incubation. Mutant and total colony count at each dose level were determined by triplicate plates.
Test substance	:	Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11). Data used as read-across to 1,2-benzenedicarboxylic acid, dinonyl ester (dinonyl phthalate). CAS# 68515-45-7.
Conclusion	:	Under conditions of this study the test substance was non-mutagenic in the mouse lymphoma assay with or without metabolic activation.
Reliability	:	(1) valid without restriction

06.11.2001

(3)

6. References

(1) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, Chemosphere 41:1389-1399.

(2) David, R., R. McKee, J. Butala, R. Barter and M. Kayser (2001), Chapter 80 - Esters of Aromatic Mono, Di and Tricarboxylic acids and Di, Tri, or Polyalcohols, Patty's Toxicology, 5th edition, Vol 6., J Wiley & Sons, Inc. pp 635-932.

(3) E. Barber, M. Cifone, J. Rundell, R. Przygoda, B. Astill, E. Moran, A. Mulholland, E. Robinson and B. Schneider. (2000). Results in the L5178Y mouse lymphoma and the in vitro transformation of Balb 3T3 cell assays for eight phthalate esters. Journal of Applied Toxicology 20:69-80.

(4) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(5) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(6) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997), the Environmental Fate of Phthalate Esters: A literature Review, Chemosphere 35:667-749.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 68515-47-9
CAS No.	:	68515-47-9
EINECS Name	:	Di-tridecyl Phthalate
EINECS No.	:	271-089-3
Molecular Weight	:	526

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - high MW phthalates
Printing date	:	12.11.2001
Revision date	:	
Date of last Update	:	12.11.2001
Number of Pages	:	16
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers:
68648-93-1
117-84-0
68515-40-2
68515-45-7
68515-43-5
84-77-5
3648-20-2
85507-79-5
111381-91-0
68515-47-9

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to

their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

2.1 MELTING POINT

Value	:	-37 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	
Remark	:	Literature review collecting data from a variety of sources. Manufacturer's data or handbook value
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

19.12.2000 (10)

Value	:	177 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation Melting point calculation seems to give erroneously high results for the phthalate esters
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(3) invalid

10.10.2001 (9)

2.2 BOILING POINT

Value	:	501 - ° C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (9)

2.4 VAPOUR PRESSURE

Value	:	.000000000363 - hPa at 25° C
Decomposition	:	no
Method		other (measured)
Year	:	2000

GLP	:	
Test substance	:	
Decomposition	:	no
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

19.12.2000 (6)

Value	:	.00000000093 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (9)

2.5 PARTITION COEFFICIENT

Log pow	:	12.06 - at 25° C
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

19.12.2000 (6)

Log pow	:	12.25 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

19.12.2000 (9)

2.6.1 WATER SOLUBILITY

Value	:	.00002 - other: ug/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000

GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001

(9)

Value	:	.00007 - other: ug/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

19.12.2000

(6)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.0000000000246 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

19.12.2000 (9)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	7.7 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

12.11.2001 (9)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	0
Water (level I)	:	0
Soil (level I)	:	97.8
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000

Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
19.12.2000 (8)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 2000
Result : Soil - 97.8%
Air - 0.0000244%
Water - 0.0000000621%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
19.12.2000 (8)

3.5 BIODEGRADATION

Type : aerobic
Inoculum : domestic sewage
Concentration : 20mg/l related to Test substance
related to
Contact time : 28 day
Degradation : = 37 - % after
Result : other
Deg. Product :
Method : other
Year : 1983
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Method : Method/Guideline-USEPA 1982, CO2 Evolution, Shake Flask (modified Gledhill).
Inoculum-Domestic sewage, soil, and mineral medium.
Kinetics-Not Reported
Degradation Products-Not Reported
Analytical Monitoring-Yes
Result : Primary degradation is expressed as the loss of initial test substance. Ultimate biodegradation is expressed as the percentage of ThCO2 in each flask.

>50% primary biodegradation occured and 37.0% (sd 10) ultimate biodegradation. The test substance was continueing to degrade at 28 days.
Test condition : Inoculum was aged for 2 weeks prior to test initiation. The test chemical was added to flasks containing medium and inoculum. The flask were incubated and shaken in the dark for 28 days. Three replicates for CO2 evaluation and 4 replicates for primary degradation were tested. The CO2 production was captured in barium hydroxide solution. Primary biodegradation was determined at the beginning, middle and end by GC FID of entire contents of one replicate. A glucose and blank were also tested..

2L Erlenmeyer flasks were used as test vessels. The pH at initiation was 7.0 to 7.2. Test flasks were shaken at a rate of 120rpm at 22 +/- 2 Deg C.

Nominal test concentration = 20mg/L for test substance and glucose.
Test substance : Ditridecyl Phthalate (CAS# 68515-47-9)
(1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters C13 rich)

Synonym: DTDP

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
28.11.2000 (11)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	m >= 1.5 -
Method	:	other
Year	:	1982
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians. Statistical methods-Moving average angle, Probit or Bionomial
Result	:	No mortality was observed in the test treatments, however one Control replicate exhibited total mortality (50% control mortality overall). Mean measured values used in calculation of LC50. Measured values remained consistent during the exposure period. Undissolved test substance was observed on the surface of the highest test treatment (1.5mg/L) on Day 0 and for the duration of exposure. Fish mean Total length=39mm, mean wet weight=0.5g
Test condition	:	Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15L of solution. The diluter maintained a water turnover rate of 5-8 tank volumes per day. Two replicates of ten organisms were tested per treatment. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection. Analytical samples taken at time zero and on a composite of replicates at termination. Test temperature=10.0 Deg C., The pH range was 6.9 to 7.3. The mean Dissolved Oxygen ranged from 10.2 to 10.4 mg/L. Fish were obtained from Montana. Nominal test concentrations: Control, 0.018, 0.036, 0.072, 0.14, and 0.29 mg/L. Mean measured test concentrations: <0.0094, 0.013, 0.023, 0.039, 0.067, and 1.5mg/L.
Test substance	:	Ditridecyl Phthalate (CAS# 68515-47-9) (1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters C13 rich) Synonym: DTDP
Conclusion	:	Test substance is non-toxic to fish at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document 1.
Reliability	:	(2) valid with restrictions Control mortality occured in the study.
Flag	:	Critical study for SIDS endpoint

12.11.2001 (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	m > .05 -
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975 Statistical methods-Moving average angle, Probit or Bionomial
Result	:	Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined slightly during study exposure in all test solutions. Lc50 value of >0.068 ppm (based upon Day 0 analytical samples) was recalculated as >0.05 ppm as per USEPA current practices of using the mean of measured initation and termination samples 1.
Test condition	:	Test treatments were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 2 minutes. Dilutions of the stock were prepared for each treatment level. The stock solution was prepared at the highest treatment concentration. Three replicates of five organisms were tested per treatment. Test vessels were 250ml beakers with 200ml of test solution. Analytical method was Gas Liquid Chromatography (GLC). Test temperature=22 +/- 2 Deg C., The pH was 8.3 at initiation and was from 8.4 at Day 2. Dissolved Oxygen ranged from 7.6 to 8.7 at initiation and 7.6 to 7.9 at Day 2. Daphnia were <24 hours old and obtained from in-house stock. Nominal test concentrations: control, 0.032, 0.055, 0.090, 0.15, and 0.25mg/L. Measured test concentrations <0.0086, <0.0086, 0.012, 0.022, 0.036, 0.069 (Day 0) Measured test concentrations <0.0090, <0.0090, <0.0090, 0.011, 0.022, 0.041 mg/L (Day 2).
Test substance	:	Ditridecyl Phthalate (DTDP, CAS# 68515-47-9) (1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters C13 rich) Synonym: DTDP
Conclusion	:	Test substance is non-toxic to Daphnid at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document.1
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

28.11.2000 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	
Exposure period	:	8 day
Unit	:	mg/l
Analytical monitoring	:	yes
EC50	:	m > .6 -
Method	:	other

Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-EPA 600/9-78-018, Printz Algal Assay Bottle Test, 1978. Test type-Static Acute Statistical methods-Moving average angle, Probit or Bionomial
Result	:	In-vivo chlorophyll a, measured daily until less than 5% change. Both cell numbers and in-vivo chlorophyll a, measured at termination. Analytical samples taken at time zero and on a composite of replicates at termination. EC50 =>1.0 ppm based upon Day 0 measured values only. Value recalculated as >0.6ppm as per USEPA current practices using the mean of measured initiation and termination samples 1.
Test condition	:	Algal Growth Medium was used as the control and diluent. 10uL of test substance was added to 1.0L of sterile water to form a saturated phthalate solution. This solution was sonicated for 1 minute and allowed to settle for 4 hours. After settling, the water soluble fraction (WSF) was removed for testing. Initial algal concentration was 2.0x104 cells/ml. Only one treatment level was evaluated (100%WSF). Based upon earlier phthalate testing, toxicity was not expected. Lighting =4,700 lux, test temperature=22+/-2 Deg C. The pH range was 7.4 at initiation and 8.4 to 8.6 at Day 8. Algal culture stock obtained from Univ. of Texas at Austin. Nominal test concentrations: 100% WSF (10ul/L stock). Measured test concentrations = 1.0 ppm on Day 0, Measured test concentration = 0.1 ppm on Day 8
Test substance	:	Ditridecyl Phthalate (CAS# 68515-47-9) (1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters C13 rich) Synonym: DTDP
Conclusion	:	Test substance is not toxic to algae at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document 1.
Reliability	:	(2) valid with restrictions Control chlorophyll or cell counts not reported.
Flag	:	Critical study for SIDS endpoint

28.11.2000

(5)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	35
Vehicle	:	no data
Value	:	> - 10000 mg/kg bw
Method	:	other
Year	:	1981
GLP	:	yes
Test substance	:	other TS
Remark	:	No rats died during the study. The animals were generally free of abnormalities throughout the observation period. There were no significant findings at the terminal sacrifice.
Test condition	:	Following a 18 hour fasting period, animals were administered the test compound at doses of 1.0, 1.47, 2.15, 3.16, 4.64, 6.81, and 10.0 mg/kg of body weight. Observations were recorded immediately after dosing, then at 1, 2, and 4 hours; and once daily thereafter for 14 days. Body weights were recorded prior to dosing and at 7 and 14 days. Gross necropsies were conducted on all animals that were sacrificed at the termination of the study.
Test substance	:	1,2-benzenetricarboxylic acid, di-C11-14-branched alkyl esters, C13 rich.
Conclusion	:	Under the conditions of this study, the test material has a low order of acute oral toxicity.
Reliability	:	(1) valid without restriction

28.12.2000 (2)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	8
Vehicle	:	no data
Value	:	> - 3160 mg/kg bw
Method	:	other
Year	:	1981
GLP	:	yes
Test substance	:	other TS
Remark	:	No rabbits died during the study. The animals in the highest dose group (3.16 g/kg) showed weight losses over the first week but all animals gained weight during the second week. Signs of skin irritation were observed during the first week, ranging from barley perceptible erythema in the lowest doses to moderate/severe erythema in the high dose group. No irritation was observed by the end of the study. There were no significant findings at the terminal sacrifice.
Test condition	:	The dose levels were 50, 200, 794, and 3160 mg/kg body weight. On the day prior to dosing the fur of each rabbit was clipped. The skin was intact and not abraded. The test material was applied directly to the skin and evenly spread; the area was wrapped with gauze and an impervious plastic sleeve. The wraps were removed after 24 hours and dermal observations recorded. General observations were recorded immediately after dosing, then at 1, 2, and 4 hours; and once daily thereafter for 14 days. Observations for skin irritation were recorded 30 minutes after removal of the wrap and at Days 3, 7, 10, and 14. Body weights were

recorded prior to dosing and at 7 and 14 days. Gross necropsies were conducted on all animals that were sacrificed at the termination of the study.

Test substance : 1,2-benzenetricarboxylic acid, di-C11-14-branched alkyl esters, C13 rich. (ditridecyl phthalate, DTDP)

Conclusion : Under the conditions of this study, the test material has a low order of acute dermal toxicity.

Reliability : (1) valid without restriction
28.12.2000

(1)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Bacterial
Concentration : 5 dose levels up to 10 mg/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year : 1985
GLP : no data
Test substance : other TS
Method : A mutagenic response was defined as a reproducible, dose-related increase in the number of histidine-independent colonies over the spontaneous incidence. There was no requirement for a specific magnitude of increase.

Test condition : Approximately 10E8 bacteria were mixed with 0.5 ml of either 0.1M sodium phosphate buffer or S-9 mix, and test substance. The reaction was carried out in triplicate. The mixture was incubated at 37°C for 48 hours, after which time histidine-revertant colonies were counted. The doses selected were separated by half-log intervals. The high dose was 10 mg/plate unless limited by solubility. Positive control chemicals were sodium azide, nitro-o-phenylenediamine, 9-aminoacridine and 2-aminoanthracene. Concurrent solvent and positive controls were included in all experiments. A toxicity pretest with TA 100 was conducted to determine the high dose level.

Test substance : 1,2-benzenetricarboxylic acid, di-C13-branched alkyl esters. (ditridecyl phthalate, DTDP)

Conclusion : No mutagenic activity was observed at doses up to 10 mg/plate in Salmonella strains TA 98, TA 100, TA 1535 and TA 1537 with or without metabolic activation.

Reliability : (1) valid without restriction
10.10.2001

(7)

(1) Bio/dynamics, Inc. (1981). Acute Dermal Toxicity in Rabbits. Conducted for Exxon Biomedical Sciences, Inc. Unpublished Report

(2) Bio/dynamics, Inc. (1981). Acute Oral Toxicity in Rats. Conducted for Exxon Biomedical Sciences, Inc. Unpublished Report.

(3) CMA Study, Acute Toxicity of Fourteen Esters to Daphnia magna., Springborn Bionomics, Inc. 1984. Report # BW-84-4-1567.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(4) CMA Study, Acute Toxicity of Fourteen Esters to Rainbow Trout Salmo gairdneri Under Flow-Through Conditions. EG&G Bionomics, Inc. 1983. Report # BW-83-3-1373, Performed Jul 1982 to Jan 1983.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(5) CMA Study, Toxicity of Fourteen Esters to the Freshwater Green Alga Selenastrum capricornutum. 1984, Springborn Bionomics, Inc. Performed 3-11 Aug 1983.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(6) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, Chemosphere 41:1389-1399.

(7) E. Zeiger, S. Haworth, K. Mortelmans, and W. Speck (1985). Mutagenicity Testing of Di(2-ethylhexyl) phthalate and Related Chemicals in Salmonella. Environmental Mutagenesis 7: 213-232.

(8) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(9) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(10) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997), the Environmental Fate of Phthalate Esters: A literature Review, Chemosphere 35:667-749.

(11) Sugatt, R.H. et al, 1983 Shake Flask Biodegradation of 14 Commercial Phthalate Esters. Syracuse Research Corporation, Syracuse, NY. SRC# L1543-05. Performed for CMA.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 68648-93-1
CAS No.	:	68648-93-1
TSCA Name	:	1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters
Synonym	:	Phthalic acid, dialkyl(C7) ester

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	09.11.2001
Revision date	:	
Date of last Update	:	10.10.2001
Number of Pages	:	14
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers:
68648-93-1
117-84-0
68515-40-2
68515-45-7
68515-43-5
84-77-5
3648-20-2
85507-79-5
111381-91-0
68515-47-9

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic

solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

2.1 MELTING POINT

Value : -45 - ° C
Remark : Manufacturer's data or handbook value
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (4) not assignable
15.12.2000 (5)

Value : 64 - ° C
Decomposition : no at - ° C
Sublimation : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Melting point calculation seems to give erroneously high results for the phthalate esters
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (3) invalid
10.10.2001 (7)

2.2 BOILING POINT

Value : 417 - ° C at 1013 hPa
Decomposition : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001 (7)

2.4 VAPOUR PRESSURE

Value : .000000131 - hPa at 25° C
Decomposition : no
Method other (measured)
Year : 2000
GLP :
Test substance :
Decomposition : no
Remark : Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (1) valid without restriction
15.12.2000 (4)

Value	:	.000000456 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (7)

2.5 PARTITION COEFFICIENT

Log pow	:	8.17 - at 25° C
Method		other (measured)
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

15.12.2000 (4)

Log pow	:	8.54 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (7)

2.6.1 WATER SOLUBILITY

Value	:	.00018 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (7)

Value	:	.00088 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

15.12.2000 (4)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.00000000002058 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (7)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	7.7 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

15.12.2000 (7)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.0064
Water (level I)	:	.0003
Soil (level I)	:	97.7
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

15.12.2000 (6)

3.3.2 DISTRIBUTION

Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level I
Year	:	2000
Result	:	Soil - 97.7% Air - 0.0064% Water - 0.00032% Sediment - 2.17% Suspended sed. - 0.068%
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (6)

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	domestic sewage
Concentration	:	20mg/l related to Test substance related to
Contact time	:	28 day
Degradation	:	= 90.3 - % after
Result	:	readily biodegradable
Deg. Product	:	
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA 1982, CO2 Evolution, Shake Flask (modified Gledhill). Inoculum-Domestic sewage, soil, and mineral medium. Kinetics-Not Reported Degradation Products-Not Reported Analytical Monitoring-Yes
Result	:	Primary degradation is expressed as the loss of initial test substance. Ultimate biodegradation is expressed as the percentage of ThCO2 in each flask. >99% primary biodegrdation and 90.3% ultimate biodegradation.
Test condition	:	Inoculum was aged for 2 weeks prior to test initiation. The test chemical was added to flasks containing medium and inoculum. The flask were incubated and shaken in the dark for 28 days. Three replicates for CO2 evaluation and 4 replicates for primary degradation were tested. The CO2 production was captured in barium hydroxide solution. Primary biodegradation was determined at the beginning, middle and end by GC FID of entire contents of one replicate. A glucose and blank were also tested. 2L Erlenmeyer flasks were used as test vessels. The pH at initiation was 7.0 to 7.2. Test flasks were shaken at a rate of 120rpm at 22 +/- 2 Deg C. Nominal test concentration = 20mg/L for test substance and glucose.
Test substance	:	Di (n-decyl, n-hexyl, n-octyl) phthalate, (CAS# 68648-93-1) (1,2,-benzenedicarboxylic acid, mixed decyl, hexyl and octyl diesters) Synonym: 610P

Conclusion : The substance is readily biodegradable using mixed populations of microorganisms,

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

29.11.2000 (8)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	m >= .24 -
Method	:	other
Year	:	1982
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians. Statistical methods-Moving average angle, Probit or Bionomial
Result	:	Mean measured values used in calculation of LC50. Analytical samples taken at time zero and on a composite of replicates at termination. Measured values remained consistent during the exposure period. No mortality was observed. Undissolved test substance was observed on the surface of the high concentration (0.24mg/L) on Day 0 and for the duration of the study. Fish mean Total length=39mm, mean wet weight=0.5g
Test condition	:	Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15L of solution. The diluter maintained a water turnover rate of 5-8 tank volumes per day. Two replicates of ten organisms were tested per treatment. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection. Test temperature=11.0 +/- 1 Deg C., The pH range was 7.0 to 7.5. The mean Dissolved Oxygen ranged from 9.7 to 9.9 mg/L. Fish were obtained from Montana. Nominal test concentrations: control, 0.018, 0.036, 0.072, 0.14, and 0.29mg/L. Mean measured test concentrations: <0.0097, 0.018, 0.030, 0.060, 0.011, and 0.24mg/L.
Test substance	:	Di (n-decyl, n-hexyl, n-octyl) phthalate, (CAS# 68648-93-1) (1,2,-benzenedicarboxylic acid, mixed decyl, hexyl and octyl diesters) Synonym: 610P
Conclusion	:	Test substance is non-toxic to fish at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document 1.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

28.11.2000 (2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)

Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	m > .33 -
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975 Statistical methods-Moving average angle, Probit or Bionomial
Result	:	Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined slightly during study exposure. More than 50% of the test organisms were trapped on the surface or air bubbles during the study (except control). LC50 value of >0.42 ppm (based upon Day 0 analyitcal samples) was recalculated as >0.33 ppm as per USEPA current practices using the mean of measured initiation and termination samples. 1
Test condition	:	Test treatments were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 2 minutes. Dilutions of the stock were prepared for each treatment level. The stock solution was prepared at the highest treatment concentration. Three replicates of five organisms were tested per treatment. Test vessels were 250ml beakers with 200ml of test solution. Analytical method was Gas Liquid Chromatography (GLC). Test temperature=22 +/- 2 Deg C., The pH was 8.3 at initiation and was from 8.4 at Day 2. Dissolved Oxygen ranged from 8.9 to 9.4 at initiation and 7.3 to 7.5 at Day 2. Daphnia were <24 hours old and obtained from in-house stock. Nominal test concentrations: control, 0.032, 0.055, 0.090, 0.15, and 0.25mg/L. Measured test concentrations <0.0091, 0.031, 0.053, 0.89, 0.14, and 0.24 (Day 0) Measured concentrations <0.010, 0.014, 0.018, 0.030, NS, 0.090mg/L (Day 2).
Test substance	:	Di (n-decyl, n-hexyl, n-octyl) phthalate, (CAS# 68648-93-1) (1,2,-benzenedicarboxylic acid, mixed decyl, hexyl and octyl diesters) Synonym: 610P
Conclusion	:	Test substance is non-toxic to Daphnia at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document.1
Reliability	:	(2) valid with restrictions Excessive test organisms trapped on surface. Excessive test organisms trapped on surface.
Flag	:	Critical study for SIDS endpoint

29.11.2000 (1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	
Exposure period	:	6 day
Unit	:	
Analytical monitoring	:	yes
EC50	:	m > .1 -

Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method/Guideline-EPA 600/9-78-018, Printz Algal Assay Bottle Test, 1978 Test type-Static Acute Statistical methods-Moving Average Angle, Probit or Binomial
Result	:	In-vivo chlorophyll a, measured daily until less than 5% change. Both cell numbers and in-vivo chlorophyll a, measured at termination. Analytical samples taken at time zero and on a composite of replicates at termination.
Test condition	:	Algal Growth Medium was used as the control and diluent. 10uL of test substance was added to 1.0L of sterile water to form a saturated phthalate solution. This solution was sonicated for 1 minute and allowed to settle for 4 hours. After settling, the water soluble fraction (WSF) was removed for testing. Initial algal concentration was 2.0x104 cells/ml. Only one treatment level was evaluated (100% WSF). Based upon earlier phthalate testing, toxicity was not expected. Lighting =4,500lux, Test temperature=22+/-2 Deg C. The pH range was 7.4 at initiation and 7.8 - 7.9 at termination. Algal culture stock obtained from Univ. of Texas at Austin. Nominal test concentrations: 100% WSF, (10ul/L). Measured test concentrations: 0.1 ppm (Day 0), Measured test concentrations: ND (Not Detected) on Day 6. Units-ppm Value-EC50 >0.1 ppm based upon cell numbers and Day 0 measured values only. Value recalculated as >0.08 ppm as per USEPA current practices using mean of measured initiation and termination samples. 1
Test substance	:	Di (n-decyl, n-hexyl, n-octyl) phthalate, (CAS# 68648-93-1) (1,2,-benzenedicarboxylic acid, mixed decyl, hexyl and octyl diesters) Synonyms: 610P
Conclusion	:	No significant toxicity was observed at or below the test substance's water solubility.
Reliability	:	(2) valid with restrictions Control chlorophyll or cell counts not reported
Flag	:	Critical study for SIDS endpoint

28.11.2000

(3)

6. References

(1) CMA Study, Acute Toxicity of Fourteen Esters to Daphnia magna., Springborn Bionomics, Inc. 1984. Report # BW-84-4-1567.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(2) CMA Study, Acute Toxicity of Fourteen Esters to Rainbow Trout Salmo gairdneri Under Flow-Through Conditions. EG&G Bionomics, Inc. 1983. Report # BW-83-3-1373, Performed Jul 1982 to Jan 1983.

1 Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(3) CMA Study, Toxicity of Fourteen Esters to the Freshwater Green Alga Selenastrum capricornutum. 1984, Springborn Bionomics, Inc. Testing performed 2-8 Nov 1983.

1Ref: Staples, C.A. et al, Aquatic Toxicity of Eighteen Phthalate Esters, 1997, Environmental Toxicology and Chemistry, Vol 16, No.5.

(4) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, Chemosphere 41:1389-1399.

(5) David, R., R. McKee, J. Butala, R. Barter and M. Kayser (2001), Chapter 80 - Esters of Aromatic Mono, Di and Tricarboxylic acids and Di, Tri, or Polyalcohols, Patty's Toxicology, 5th edition, Vol 6., J Wiley & Sons, Inc. pp 635-932.

(6) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(7) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(8) Sugatt, R.H. et al, 1983 Shake Flask Biodegradation of 14 Commercial Phthalate Esters. Syracuse Research Corporation, Syracuse, NY. SRC# L1543-05. Performed for CMA.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 84-77-5
CAS No.	:	84-77-5
TSCA Name	:	1,2-benzenedicarboxylic acid, didecyl ester
Generic name	:	didecyl phthalate
Molecular Formula	:	C28H46O4

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - high MW phthalates
Printing date	:	12.11.2001
Revision date	:	
Date of last Update	:	12.11.2001
Number of Pages	:	10
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers:
68648-93-1
117-84-0
68515-40-2
68515-45-7
68515-43-5
84-77-5
3648-20-2
85507-79-5
111381-91-0
68515-47-9

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to

their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

2.1 MELTING POINT

Value	:	<= 48 - ° C
Sublimation	:	
Method	:	other: unknown
Year	:	
GLP	:	no
Test substance	:	
Remark	:	Literature review collecting data from a variety of sources, including Manufacturer's data or handbook value.
Reliability	:	(4) not assignable

12.11.2001 (4)

Value	:	136 - ° C
Decomposition	:	no at - ° C
Sublimation	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation Melting point calculation seems to give erroneously high results for the phthalate esters
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(3) invalid

10.10.2001 (3)

2.2 BOILING POINT

Value	:	477 ° C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

10.10.2001 (3)

2.4 VAPOUR PRESSURE

Value	:	.0000000105 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation

method of Grain.

Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
10.10.2001 (3)

Value : .0000000184 - hPa at 25° C
Decomposition : no
Method other (measured)
Year : 2000
GLP :
Test substance :
Decomposition : no
Remark : Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (1) valid without restriction
15.12.2000 (1)

2.5 PARTITION COEFFICIENT

Log pow : 9.461 - at 25° C
Method other (measured)
Year : 2000
GLP :
Test substance :
Remark : Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (1) valid without restriction
12.11.2001 (1)

Log pow : 10.5 - at 25° C
Method other (calculated)
Year : 2000
GLP :
Test substance :
Method : Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
15.12.2000 (3)

2.6.1 WATER SOLUBILITY

Value : .00004 - mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Method : other
Year :
GLP :
Test substance :
Remark : Measured data collected and tabulated, calculated data also considered in determining recommended values.

Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction
15.12.2000		(1)
Value	:	.00168 - other: ug/L at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions
12.11.2001		(3)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.2623 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (3)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	7.7 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

15.12.2000 (3)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	.0002
Water (level I)	:	0
Soil (level I)	:	97.8
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

Reliability : (2) valid with restrictions
15.12.2000 (2)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 2000
Result : Soil - 97.8%
Air - 0.0000035%
Water - 0.0002%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
19.12.2000 (2)

6. References

(1) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, Chemosphere 41:1389-1399.

(2) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(3) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(4) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997). The environmental fate of phthalate esters: A literature review. Chemosphere 35: 667-749.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 85507-79-5
CAS No.	:	85507-79-5
EINECS Name	:	Diundecyl phthalate
EINECS No.	:	287-401-6
TSCA Name	:	1,2-Benzenedicarboxylic acid, diundecyl ester, branched and linear
Molecular Weight	:	474
Molecular Formula	:	C3OH5OO4

Producer Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance Related Part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - high MW phthalates
Printing date	:	12.11.2001
Revision date	:	
Date of last Update	:	12.11.2001
Number of Pages	:	10
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

02.11.2001

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	- % w/w

02.11.2001

1.1.0 DETAILS ON TEMPLATE

Comment

This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following ten CAS numbers:
68648-93-1
117-84-0
68515-40-2
68515-45-7
68515-43-5
84-77-5
3648-20-2
85507-79-5
111381-91-0
68515-47-9

Remark

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic

solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Ten of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

2.1 MELTING POINT

Value : -9 - ° C
Decomposition : no at - ° C
Sublimation : no
Method :
Year :
GLP :
Test substance :
Remark : Literature review collecting data from a variety of sources.
Manufacturer's data or handbook value
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
19.12.2000 (5)

Value : 142 - ° C
Sublimation : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Melting point calculation seems to give erroneously high results for the phthalate esters
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (3) invalid
08.10.2001 (4)

2.2 BOILING POINT

Value : 499 ° C at 1013 hPa
Decomposition : no
Method : other
Year : 2000
GLP :
Test substance :
Method : Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
08.10.2001 (4)

Value : 270 ° C at 1013 hPa
Decomposition : no
Method : other
Year : 2000
GLP :
Test substance :
Remark : Manufacturer's data or handbook value.
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (4) not assignable
08.10.2001 (2)

2.4 VAPOUR PRESSURE

Value	:	.00000000271 - hPa at 25° C
Decomposition	:	no
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	no
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

08.10.2001 (4)

Value	:	.00000000497 - hPa at 25° C
Decomposition	:	no
Method		other (measured)
Year	:	
GLP	:	
Test substance	:	
Decomposition	:	no
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

19.12.2000 (1)

2.5 PARTITION COEFFICIENT

Log pow	:	10.33 - at 25° C
Method		other (measured)
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

12.11.2001 (1)

Log pow	:	11.83 - at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

12.11.2001 (4)

2.6.1 WATER SOLUBILITY

Value	:	.00007 - other: ug/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

08.10.2001 (4)

Value	:	.00441 - other: ug/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Remark	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(1) valid without restriction

19.12.2000 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	- nm
Rel. intensity	:	1 - based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	.00000000003185 cm3/(molecule*sec)
Degradation	:	- % after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

19.12.2000 (4)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	- at degree C
t1/2 pH7	:	6.3 - year at 25 degree C
t1/2 pH9	:	- at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

19.12.2000 (4)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	other
Air (level I)	:	0
Water (level I)	:	0
Soil (level I)	:	97.8
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000

Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
08.10.2001 (3)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 2000
Result : Soil - 97.8%
Air - 0.0000654%
Water - 0.000000163%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
12.11.2001 (3)

6. References

(1) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, Chemosphere 41:1389-1399.

(2) David, R., R. McKee, J. Butala, R. Barter and M. Kayser (2001), Chapter 80 - Esters of Aromatic Mono, Di and Tricarboxylic acids and Di, Tri, or Polyalcohols, Patty's Toxicology, 5th edition, Vol 6., J Wiley & Sons, Inc. pp 635-932.

(3) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(4) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(5) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997), the Environmental Fate of Phthalate Esters: A literature Review, Chemosphere 35:667-749.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

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Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT