ExxonMobil Chemical Company
13501 Katy Freeway
Houston, TX 77079-1398
281.870.6783 Telephone
281.588 4664 Facsimile

Nigel J. Sarginson
Manager
Product Stewardship & Regulatory Affairs
Intermediates Americas

ExxonMobil
Chemical

Via Electronic Submission
February 5, 2002

Hon. Christine Todd Whitman
US Environmental Protection Agency
PO Box 1473
Merrifield, VA 22116

Attn: Chemical Right-to-Know Program
ExxonMobil Chemical Company Registration Number

Dear Ms. Whitman:

ExxonMobil Chemical Company (EMCC) has previously submitted for review and public comment the test plan and related robust summaries for the *Alkyl Alcohols C6-C13* category, under the US High Production Volume (HPV) Chemical Challenge program, AR-201. We hereby submit an addendum to the test plan. The test material in an oral repeated dose study was inadvertently reported as CAS# 68526-86-3, Alcohols C11-14 iso, C13 rich. The test material was in fact the ethoxylated form of the material. The ethoxylated form of the tridecyl alcohol is not expected to be metabolized to the parent compound, so the material is not appropriate for readacross. The addendum reflects this change. However, we are including a reference to a repeated dose study that was conducted on 1-dodecanol (CAS# 112-53-8), an isomer of CAS# 68526-86-3: Alcohols C11-14 iso, C13 rich. This study is included in the European Chemicals Bureau IUCLID file that is publicly available, and was included with our original submission.

As discussed in the revised test plan, since there are publicly available repeated dose studies on isomers of the Alkyl Alcohols, no further repeated dose studies are proposed. This test plan covers the following category of chemicals, Alkyl Alcohols C6-C13:

CAS# 68526-79-4: Hexanol, branched and linear
CAS# 70914-20-4: Alcohols C6-8, branched
CAS# 68526-83-0: Alcohols C7-9 iso, C8 rich
CAS# 68526-84-1: Alcohols C8-10 iso, C9 rich
CAS# 68526-85-2: Alcohols C9-11 iso, C10 rich
CAS# 68526-86-3: Alcohols C11-14 iso, C13 rich

We understand that this information will be posted on the internet for a 120 day comment period. Please forward technical comments on this test plan to Laura H. Keller at the above address or you may contact her at (281) 870-6501 (email: laura.h.keller@exxonmobil.com).

Sincerely,

Nigel J. Sarginson
Product Stewardship & Regulatory Affairs Manager
ExxonMobil Chemical Company

AR201-13590A

HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For The

ALKYL ALCOHOLS C6 - C13 CATEGORY

CAS# 68526-79-4: Hexanol, branched and linear
CAS# 70914-20-4: Alcohols C6-8, branched
CAS# 68526-83-0: Alcohols C7-9 iso, C8 rich
CAS# 68526-84-1: Alcohols C8-10 iso, C9 rich
CAS# 68526-85-2: Alcohols C9-11 iso, C10 rich
CAS# 68526-86-3: Alcohols C11-14 iso, C13 rich

RECEIVED
OPPT NCIC
02 FEB -6 AM 9:57

Prepared by:

ExxonMobil Chemical Company

November 15, 2001

(Revised February 5, 2002)

EXECUTIVE SUMMARY

Under EPA's High Production Volume (HPV) Chemical Challenge Program, ExxonMobil Chemical Company has committed to voluntarily compile a Screening Information Data Set (SIDS) on a category of chemicals defined as Alkyl Alcohols C6 - C13. This category is supported by the basic screening data needed for an initial assessment of the physicochemical properties, environmental fate, and human and environmental effects of chemicals as defined by the Organization for Economic Cooperation and Development (OECD). The information used to complete the HPV SIDS endpoints comes from existing data.

ExxonMobil Chemical Company believes a category of Alkyl Alcohols C6 - C13 is scientifically justifiable because their physicochemical and toxicological properties are very similar and follow a regular pattern as a result of the synthesis process. The structural similarity of the component chemicals from these products creates a predictable pattern in the following parameters: physicochemical properties, environmental fate and environmental effects, and human health effects. The similarities are based on the following:

- A common structure represented by RCOH,
- An incremental and constant change across the category where R is a branched alkyl group having carbon numbers C5, C6, C7, C8, C9, C11, or C12 as the main constituent, and
- A likelihood of common precursors and breakdown products that can result in structurally similar metabolites (e.g. carboxylic acid).

This test plan is based on the observation that the toxicological properties are similar or vary in an incremental and predictable fashion within the category.

The test data compiled for the category anchor studies proves adequate to support a screening-level hazard assessment for the category and its members (CAS numbers, 68526-79-4, 70914-20-4, 68526-83-0, 68526-84-1, 68526-85-2, and 68526-86-3). The untested endpoints can be assessed by interpolation between data from the category anchor studies.

Substantial amounts of data exist to evaluate selected potential hazards of Alkyl Alcohols C6-C13. To complete the health hazard assessment of the category, a mouse micronucleus assay will be conducted on Alkyl Alcohol C6 and compared to clastogenicity data on other category members. The ecological hazard assessment will be completed by conducting an acute algal toxicity study on the C6 (68526-79-4) and C13 (68526-86-3) alkyl alcohols.

Evaluation of the Alkyl Alcohols C6 - C13 as a category has several advantages. All products in this category can be adequately characterized for the HPV endpoints by using a matrix of completed studies for members in the category. By using this approach, the safety of the category can be determined without having to conduct tests for every endpoint with every chemical. Not only will this inform the public about the potential hazards of Alkyl Alcohols C6 - C13, but it will also reduce the number of animals that would be required to evaluate the toxicity of individual members of the Alkyl Alcohols C6 - C13 Category.

TABLE OF CONTENTS

	Page
EXECUTIVE SUMMARY	2
I. INTRODUCTION	4
II. CHEMICAL AND PROCESS DESCRIPTION OF THE ALKYL ALCOHOLS C6 - C13 CATEGORY	5
Table 1. CAS Numbers and Descriptions	5
III. TEST PLAN RATIONALE	6
A. Physicochemical Data	6
Table 2. Physical Properties of Alkyl Alcohols C6 - C13	6
B. Human Health Effects	7
C. Presentation of Alkyl Alcohols C6 - C13 Category Data Associated with the Anchor Studies under the HPV Challenge Program	8
D. Aquatic Toxicity	14
E. Environmental Fate	16
IV. TEST PLAN SUMMARY	19
REFERENCES	20
Table 3. Assessment Plan for the Alkyl Alcohols C6-C13 Category Under the Program.	24

TEST PLAN FOR ALKYL ALCOHOLS C6 - C13

I. INTRODUCTION

Under EPA's High Production Volume (HPV) Chemical Challenge Program, ExxonMobil Chemical Company has committed to voluntarily compile a Screening Information Data Set (SIDS) on a category of chemicals defined as Alkyl Alcohols C6 - C13. This category is supported by the basic screening data needed for an initial assessment of the physicochemical properties, environmental fate, and human and environmental effects of chemicals as defined by the Organization for Economic Cooperation and Development (OECD). The information used to complete the SIDS endpoints comes from existing data and fulfills an ExxonMobil obligation to the HPV Challenge Program.

ExxonMobil Chemical Company believes a category of Alkyl Alcohols C6 - C13 is scientifically justifiable because their physicochemical and toxicological properties are very similar and follow a regular pattern as a result of the synthesis process. The structural similarity of the component chemicals from these products creates a predictable pattern in the following parameters: physicochemical properties, environmental fate and effects, and human health effects. The similarities are based on the following:

- A common structure represented by RCOH,
- An incremental and constant change across the category where R is a branched alkyl group having carbon numbers C5, C6, C7, C8, C9, C11, or C12 as the main constituent, and
- A likelihood of common precursors and breakdown products that can result in structurally similar metabolites (e.g. carboxylic acid).

This test plan is based on the observation that the toxicological properties are similar or vary in an incremental and predictable fashion within the category.

The test data compiled for the category proves adequate to support a screening-level hazard assessment for the category and its members (CAS numbers, 68526-79-4, 70914-20-4, 68526-83-0, 68526-84-1, 68526-85-2, and 68526-86-3). The untested endpoints can be assessed by interpolation between data from the category anchor studies. The existing data suggest that products in the Alkyl Alcohols C6 - C13 Category exhibit relatively low toxicity for human health endpoints and moderate to high toxicity for the environmental health endpoints.

A substantial amount of data exists to evaluate the potential hazards of Alkyl Alcohols C6-C13. To complete the health hazard assessment of the category, a mouse micronucleus assay will be conducted on Alkyl Alcohol C6 and compared to clastogenicity data on other category members. The ecological hazard assessment will be completed by conducting an acute algal toxicity study on the C6 (68526-79-4) and C13 (68526-86-3) alkyl alcohols.

The data from this category will be used to inform the public about the potential hazards of the Alkyl Alcohols C6 - C13. Developing a data matrix of anchor studies and applying justifiable read across practices will provide a sufficiently robust data set to

characterize each endpoint in the HPV Chemical Challenge Program without having to conduct a test for each endpoint and product. This resourceful use of existing data will result in fewer animals needed for testing purposes while adequately assessing the potential hazards of products in the Alkyl Alcohol C6 - C13 Category.

II. CHEMICAL PROCESS AND DESCRIPTION

The Alkyl Alcohols C6 - C13 Category contains a group of alkyl alcohol products whose physicochemical and toxicological properties are very similar and follow a regular pattern as a result of synthesis and structural similarity (Table 1). The production of alkyl alcohol products involves the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol.

The structural similarity of chemcials in the products of this category creates a predictable pattern in the following parameters: physicochemical properties, environmental fate and effects, and human health effects. The structural features of members of the category are as follows:

- A common structure - ROH,
- An incremental and constant change across the category where R is a branched alkyl group having carbon numbers of C6, C7, C8, C9, C10, C12, or C13 as the main constituent,
- A common functional hydroxyl group, and
- A likelihood of common precursors and breakdown products which result in structurally similar chemicals (e.g., carboxylic acid).

Table 1. CAS Numbers and Descriptions

CAS Number	Chemical Name	Generic Name
68526-79-4	Hexanol, branched and linear	Hexyl alcohol
70914-20-4	Alcohols C6-8, branched	Isoheptyl alcohol
68526-83-0	Alcohols C7-9, branched*	Isooctyl alcohol
68526-84-1	Alcohols C8-10 iso, C9 rich	Isononyl alcohol
68526-85-2	Alcohols C9-11 iso, C10 rich	Isodecyl alcohol
68526-86-3	Alcohols C11-14 iso, C13 rich	Tridecyl alcohol

* = Not currently HPV but included to facilitate category evaluation

Evaluation of the Alkyl Alcohols C6 - C13 as a category accomplishes the goal of the HPV Program - to obtain screening level hazard information - through the strategic selection of products within this category. The testing strategy is based on the principle that:

- These products behave in a similar and/or predictable manner, and
- Interpolation of data can be used to assess the alkyl alcohol products for which data are not available.

Procedures to assess the reliability of selected studies described in this test plan are based on the guidelines described by Klimisch *et al.*, 1997.

III. TEST PLAN RATIONALE

A. Physicochemical Data

Physicochemical data (i.e., melting point, boiling point, vapor pressure, water solubility, and Kow) for selected chemical components in the Alkyl Alcohol C6 - C13 category will be calculated using the EPIWIN© model (EPIWIN, 1999), as discussed in the EPA document titled "The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program." These data will be presented as ranges, based on the chemical components selected to represent each alkyl alcohol product. In addition, measured data for some of these endpoints will also be provided for selected alkyl alcohol products where readily available. Where possible, the measured and calculated data will be presented together for comparative purposes.

Table 2 lists selected measured physicochemical data (boiling range, vapor pressure, and specific gravity) as they appear on the material safety data sheets for products in this category. These data are provided with this test plan to further justify these products as a distinct category under the HPV Program. Also included are calculated and measured values for water solubility and K_{ow}. As shown by the data in Table 2, the structural similarity of the alkyl alcohol products results in a predictable and incrementally increasing pattern of physiochemical properties from the C6 to C13 rich products.

Table 2. Selected Physical Properties of Alkyl Alcohols C6 - C13

CAS NUMBER	CHEMICAL NAME	BOILING RANGE (° C)	VAPOR PRESSURE (mm Hg @ 100° C)	SPECIFIC GRAVITY	WATER SOLUBILITY (Mg/L)	LOG K_{ow}
68526-79-4	Hexanol, branched and linear	152 - 163	124	0.82	10,340 - 11,950[a]	1.8 - 2.0[a]
70914-20-4	Alcohols C6-8, branched	167 - 176	78	0.83	3,539 - 11,950[a]	1.8 - 2.6[a]
68526-83-0	Alcohols C7-9, branched*	185 - 193	27	0.83	1,379 - 1,485[a]	2.9 - 3.4[b]
68526-84-1	Alcohols C8-10 iso, C9 rich	203 - 215	16	0.84	164 - 614[a]	3.4 - 3.9[b]
68526-85-2	Alcohols C9-11 iso, C10 rich	217 - 224	8.2	0.84	75.0[b]	3.8[b]
68526-86-3	Alcohols C11-14 iso, C13 rich	256 - 266	2.7	0.84	5.8[b]	4.2 - 5.0[b]

* = Not currently HPV but included to facilitate category evaluation
[a] Calculated using EPIWIN
[b] Measured values (Robust summaries are attached)

B. Human Health Effects

ExxonMobil Chemical Company believes the category of Alkyl Alcohols C6 - C13 is scientifically justifiable. Furthermore, we believe that the test data compiled for the category proves adequate to support a screening-level hazard assessment of potential health hazards for the category and its members (CAS numbers, 68526-79-4, 70914-20-4, 68526-83-0, 68526-84-1, 68526-85-2, and 68526-86-3). Table 3 summarizes the proposed test plan for the category. Because of the common structure and predictable toxicity of members of the category, one can assess the untested endpoints by extrapolation between and among the category members.

Metabolism

Alkyl Alcohols would likely be broken down by mitochondrial beta-oxidation or by cytochrome P450 mediated omega and omega-minus-one oxidation (may be followed by beta-oxidation). The alcohol undergoes various oxidative steps to yield other alcohols, ketones, aldehydes, carboxylic acids and carbon dioxide (Mann, 1987). Data for monohydric, aliphatic alcohols show a systematic variation according to molecular weight in a manner similar to many other homologous series (Monick, 1968). The body handles aliphatic hydrocarbons in a similar manner via oxidative conversion to alcohols, ketones, and eventual elimination as carbon dioxide and carboxylic acids (Wislocki et al, 1980). The undegraded alcohols can be conjugated either directly or as a metabolite with glucuronic acid, sulfuric acid, or glycine and are rapidly excreted (Lington and Bevan, 1994). Intermediate aldehydes could be reactive and bind with DNA and/or proteins. Glucuronidation and glutathione conjugation are possible means of rapid elimination (Mann, 1987).

C. Presentation of Alkyl Alcohols C6 - C13 Category Health Effects Data Associated with the Anchor Studies under the HPV Challenge Program

Acute Oral Toxicity

TEST	Hexanol, branched and linear	Alkyl alcohol C6-8, branched	Alkyl alcohol C7-9, branched	Alkyl alcohol C8-10, branched	Alkyl alcohol C9-11, branched	Alkyl alcohol C11-14, branched
ACUTE ORAL - RAT	=3.7 g/kg (Hazleton, 1960)	>3.9 g/kg (Esso, 1979a)	>2 g/kg (RCC, 1988a)	=3.0 g/kg (Esso, 1968b)	=4.6 g/kg (Esso, 1960a)	>2 g/kg (RCC b,c)

All of the Alkyl Alcohols C6 - C13 have a low order of toxicity to rats via the oral route of exposure. The LD_{50} for the C6 branched and linear alkyl alcohol anchor study was >3.7 g/kg. The LD_{50}'s for the C6-C8, C7-C9, C8-C10, C9-C11, and C11-C14 branched alkyl alcohols were all > 2 g/kg. For all members of the category, acute oral exposure induced signs of systemic toxicity that were characterized by depression, sedation, and ataxia. These results demonstrate that members of the alkyl alcohol category have a consistent, low order of acute oral toxicity.

Acute Dermal Toxicity

TEST	Hexanol, branched and linear	Alkyl alcohol C6-8, branched	Alkyl alcohol C7-9, branched	Alkyl alcohol C8-10, branched	Alkyl alcohol C9-11, branched	Alkyl alcohol C11-14, branched
ACUTE DERMAL - RABBIT	>2.6 g/kg (Hazleton, 1960)	>3.16 g/kg (Esso, 1979b)	>2.6 g/kg (Hazleton, 1960)	>3.16 g/kg (Esso, 1968c)	>2.6 g/kg (Esso, 1960b)	RA

The Alkyl Alcohols C6 - C13 have a low order of toxicity via the dermal route of exposure. The rabbit dermal LD_{50} for all members of the category was greater than 2.6 g/kg. This indicates that the members of this category have a consistent pattern of acute toxicity via the dermal route of exposure.

Genotoxicity

TEST	Hexanol, branched and linear	Alkyl alcohol C6-8, branched	Alkyl alcohol C7-9, branched	Alkyl alcohol C8-10, branched	Alkyl alcohol C9-11, branched	Alkyl alcohol C11-14, branched
AMES - S. typhimurium; TA98, 100, 1535, 1537, 1538 ± Activation	NEGATIVE (1-hexanol) (ECB, 2000a)	RA	NEGATIVE (2-ethyl-1-hexanol) (Shimizu, 1985, ECB, 2000b)	RA	RA	NEGATIVE (1-dodecanol) (ECB, 2000c)
Chromosomal Aberration - In Vitro or In Vivo	ND	ND	NEGATIVE (2-ethyl-1-hexanol) (ECB, 2000b)	ND	ND	NEGATIVE (1-dodecanol) (ECB, 2000c)

RA Read Across
ND No Data

In Vitro

An evaluation of the genotoxic potential of Alkyl Alcohols C6 - C13 is based on the existing data for structural isomers as well as on data from metabolic precursors. The weight of evidence from this existing data supports the conclusion that these materials are not genotoxic and obviates the need for further testing.

Existing data on 1-hexanol, which is an isomer of Alkyl Alcohol C6, indicates that this material is not genotoxic. In addition, 2-ethyl-1-hexanol and 1-dodecanol were evaluated in Ames Assays in the presence and absence of metabolic activation. The 2-ethyl-1-hexanol is an isomer of Alkyl Alcohol C7-C9, and the 1-dodecanol is an isomer of Alkyl Alcohol C11-C14. Both materials were not mutagenic in Ames assays using five strains of *Salmonella typhimurium*. IUCLID files for 1-hexanol, 2-ethyl-1-hexanol, and 1-dodecanol are publicly available in the European Chemicals Bureau (ECB) IUCLID database and are included with this submission (ECB, 2000).

Further data to support the hazard assessment for the category comes from a series of Alkyl Acetates C6-C13. These materials have also been shown to be non-genotoxic in the Ames assay (EBSI, 1995a; 1994b,c). Alkyl Acetates are manufactured from the Alkyl Alcohols and undergo metabolism by esterases to produce acetic acid and the corresponding Alkyl Alcohol. As indicated in a previous test plan submitted for the Alkyl Acetates, there is no evidence for genotoxicity with these compounds in a variety of strains of *S. typhimurium* in the presence or absence of metabolic activation. The C6, C6-C8, C7-C9, and C11-C14 Alkyl Acetates, all of which are metabolized to the corresponding Alkyl Alcohol, produced negative results in the Ames test. These data, in conjunction with the negative data on structural isomers of these materials provide strong evidence that Alkyl Alcohols are not genotoxic.

In Vivo

Based on existing data for structurally similar materials, members of the Alkyl Alcohols C6 -C13 category are not expected to be clastogenic. However, while sufficient evidence exists for the higher molecular weight members of the Alkyl Alcohols C6 -C13 category, there is less evidence for the lack of clastogenic activity for the low molecular weight members (i.e. Alkyl Alcohol C6). Therefore, to complete the category evaluation, we will conduct a mouse micronucleus assay on Alkyl Alcohol C6 (68526-79-4). This result will be compared to the results to clastogenicity tests already conducted on structural isomers and similar materials.

In a mouse micronucleus assay, 1-dodecanol produced negative results. Furthermore, 2-ethyl-1-hexanol produced negative results in both a mouse micronucleus assay and a mouse lymphoma assay. In addition, 1-hexanol and 2-ethyl-1-hexanol were not oncogenic in chronic studies. IUCLID files for 1-hexanol, 2-ethyl-1-hexanol, and 1-dodecanol are publicly available in the European Chemicals Bureau (ECB) IUCLID database and are included with this submission (ECB, 2000).

As described before, the Alkyl acetates can be used to predict the clastogenic potential of the Alkyl Alcohols. These materials are metabolized to the corresponding alcohol. An Alkyl Acetate ester (C6) was not clastogenic in an *in vitro* chromosome aberration assay

in CHO cells (EBSI, 1995b). In addition, both a C7-C9 and C11-C14 Alkyl Acetate produced negative results in a mouse micronucleus assay (EBSI, 1994 d,e). Although there was evidence of cytotoxicity at extremely high doses, no clastogenic activity was observed. These results demonstrate that the Alkyl Acetates are not clastogenic and that they display a consistent pattern of toxicity when clastogenicity is evaluated as an endpoint.

Given the consistent pattern of toxicity displayed by members of the Alkyl Alcohol family, we feel that it is not necessary to systematically evaluate the clastogenicity of all members of the Alkyl Alcohol category. Therefore, we feel it will be sufficient to conduct a mouse micronucleus test on Alkyl Alcohol C6 and compare the results of that test to the results of tests on other Alkyl Alcohol isomers and with the Alkyl Acetates. This strategy also addresses concerns of animal welfare by reducing the number of animals required to evaluate the category.

Subchronic Toxicity

TEST	Hexanol, branched and linear	Alkyl alcohol C6-8, branched	Alkyl alcohol C7-9, branched	Alkyl alcohol C8-10, branched	Alkyl alcohol C9-11, branched	Alkyl alcohol C11-14, branched
ORAL - Rat	NOAEL (rat, dog) ≥ 0.5% in diet (ECB, 2000a) Repeat Dermal Application* NOAEL = 2.0 g/kg/day (Esso, 1961a)	RA	Subacute gavage* NOAEL = 130 mg/kg/day; (Rhodes, 1984) Subchronic gavage NOEL = 125 mg/kg/day; LOEL = 250 mg/kg/day (ECB, 2000b) Repeat Dermal Application* NOAEL = 2.0 g/kg/day (Esso, 1961b)	Subacute gavage* NOAEL = 144 mg/kg/day (Rhodes, 1984)	RA	Subchronic Feed NOEL = 100 mg/kg/day (1-dodecanol, ECB 2000c)

* Referenced Supportive Internal Study Document (Reliable with restrictions)

An evaluation of the publicly available repeated dose studies indicates that Alkyl Alcohols C6 - C13 have a low order of subchronic toxicity. Subchronic toxicity data on 1-hexanol, an isomer of Alkyl Alcohol C6, indicates that this material has a low order of subchronic toxicity. Thirteen-week dietary feeding studies in both the rat and dog produced a NOAEL greater than or equal to 0.5% in the diet. Furthermore, a number of studies have evaluated the toxicity of repeated exposure to 2-ethylhexanol, an isomer of Alkyl Alcohol C7-9. In a 3-month study in rats, 2-ethylhexanol was administered by oral gavage at doses of 25, 125, 250, and 500 mg/kg/day. At the highest doses (250 and 500 mg/kd/day), changes in body and organ weights were observed. The NOEL for the study was 125 mg/kg/day and the LOEL for the study was 250 mg/kg/day based on body weight changes. Finally, an OECD 422 oral feed study on 1-dodecanol at doses of 100, 500, and 2000 mg/kg/day produced a NOEL of 100 mg/kg/day based on a

reduction in mean white blood cell count. However, no other effects were observed in gross or histological examinations. Summaries of the subchronic studies on 1-hexanol, 2-ethylhexanol, and 1-dodecanol are publicly available from the European Chemicals Bureau (ECB) IUCLID database and are included with this submission (ECB, 2000).

A 14-day oral study was conducted in Wistar rats with iso-octanol and isononanol at doses of 130 mg/kg/day and 144 mg/kg/day, respectively. Plasma cholesterol and triglycerides were analyzed, the testes and liver were weighed, and the liver was analyzed for both histopathological lesions and the activity of peroxisomal enzymes. No treatment-related effects were observed during the study. Neither iso-octanol nor isononanol induced any significant changes in testes or liver weight, vacuolation, or activity of the peroxisome-associated enzymes. The NOAEL for iso-octanol was the limit dose of 130 mg/kg/day and the NOAEL for isononanol was the limit dose of 144 mg/kg/day.

Dermal exposure of rats to 0.4 and 2.0 g/kg/day hexyl alcohol or Alkyl alcohol C7 - 9, branched for 10 days resulted in no clinical signs of toxicity at any time during the study. All animals survived to study termination and there were no treatment-related clinical, in-life, gross postmortem or microscopic findings. The no observable adverse effect level (NOAEL) for repeat dermal exposure was 2.0 g/kg/day.

Taken together, the results of these studies demonstrate that Alkyl Alcohols C11-C14 have a low order or toxicity under conditions of repeat exposure by both the oral and dermal routes. In addition, they demonstrate that the members of the category display a consistent degree of subchronic toxicity by either the oral or dermal routes of exposure. Therefore, Alkyl Alcohols C6-C13 do not require further testing to assess subchronic toxicity.

Developmental Toxicity

TEST	Hexanol, branched and linear	Alkyl alcohol C6-8, branched	Alkyl alcohol C7-9, branched	Alkyl alcohol C8-10, branched	Alkyl alcohol C9-11, branched	Alkyl alcohol C11-14, branched
ORAL - Rat	(Inhalation) NOAEL = 3500 mg/m^3 (Nelson, 1989)	RA	DEV-TOX MATERNAL NOAEL = 500 mg/kg; FETAL NOAEL = 1000 mg/kg; (EBSI, 1994a) DEV-TOX (Inhalation) NOAEL = 400 mg/m^3 (Nelson, 1990)	DEV-TOX MATERNAL/ FETAL NOAEL = 144 mg/kg; (USEPA, 1989) DEV-TOX (Inhalation) NOAEL = 150 mg/m^3 (Nelson, 1990)	DEV-TOX MATERNAL NOAEL = 158 mg/kg; FETAL NOAEL = 790 mg/kg (USEPA, 1989b) DEV-TOX MATERNAL/ FETAL NOAEL = 1,440 mg/kg (USEPA, 1989b) DEV-TOX (Inhalation) NOAEL = 100 mg/m^3 (Nelson, 1990)	RA

*Referenced Supportive Internal Study Document (Reliable with restrictions)

Oral Exposure

Studies on the developmental toxicity of Alkyl Alcohols C6-C13 indicate that these materials have a lower order of toxicity and are not considered selective developmental toxicants by either the oral or inhalation routes of exposure. Alkyl alcohol C7-9, branched was orally administered at 100, 500, and 1000 mg/kg on gestation days 6-15 in a developmental toxicity study in rats. Maternal toxicity was seen in the high dose group as indicated by emaciation, rales, and hypoactivity. However, no adverse maternal effects were observed in the low or mid-dose groups. In addition, there were no significant signs of fetal toxicity in any of the dose groups. A maternal NOAEL of 500 mg/kg and a fetal NOAEL of 1000 mg/kg were observed.

In another study, the developmental toxicity of isononylalcohol 1 and isononylalcohol 2 were evaluated in Wistar rats. Isononyl 1 consists of isomers with a moderate degree of branching (dimethyl heptanols) and contains approximately 16% isodecanol. Isononyl 2 consists of isomers with a low degree of branching (dimethyl heptanols and methyl octanols). Each test substance was administered by oral gavage at 144, 720, or 1440 mg/kg/day during days 6-15 of gestation. At the middle and high dose levels of isononylalcohol 1, signs of maternal and fetal toxicity, including decreased body weight, were observed. At the lowest dose of isononylalcohol 1, no maternal toxicity was observed. There were an increased number of fetuses with hydroureter. However, the significance of this endpoint as an indicator of marginal developmental toxicity is questionable. Therefore, isononylalcohol 1 was considered to induce developmental toxicity only at doses that induce overt maternal toxicity. Isononylalcohol 2 also

produced maternal and fetal effects at both the middle and high doses. At the lowest dose however, no maternal or fetal toxicity was observed. Therefore, isononylalcohol 2 induced fetal toxicity at doses that also induce overt maternal toxicity. The maternal NOAEL for isononylalcohol 1 and isononylalcohol 2 is 144 mg/kg. The fetal NOAEL for isononylalcohol 1 is less than 144 mg/kg, whereas the fetal NOAEL for isononylalcohol 2 is 144 mg/kg.

In a similar study, the developmental toxicity of isodecanol (isomers of trimethyl heptanols and dimethyl octanols) was evaluated in Wistar rats by oral gavage at doses of 158, 790, and 1580 mg/kg during days 6-15 of gestation. Signs of compound-induced toxicity including reduced body weight were observed in dams of the middle and high dose groups. No maternal signs of toxicity were observed in the low dose group. Fetotoxic effects including reduced mean fetal body weight and skeletal retardations were observed only in the highest dose group. The maternal NOAEL for this study was 158 mg/kg and the fetal NOAEL was 790 mg/kg. Thus, isodecanol is fetotoxic only at doses that produce overt maternal toxicity.

An identical study conducted concurrently on C-7-9-11 alcohol (consists of isomers of heptanol, nonanol, and undecanol) produced negative results at all three dose levels tested: 144, 720, and 1440 mg/kg/day. No adverse effects were observed in dams or in the fetuses at any of these doses. The NOAEL for this study was therefore 1440 mg/kg/day.

Inhalation Exposure

The developmental toxicity resulting from inhalation of saturated vapors has also been evaluated for several members of the Alkyl Alcohols C6 - C13 category. Inhalation of Alkyl Alcohols C6-C13 is the primary concern during industrial use, particularly for the lower molecular weight members of the category. Therefore, an evaluation of inhalation studies is useful for evaluating the developmental toxicity of the category.

The available developmental toxicity data for structural isomers of the Alkyl Alcohols indicate that these materials are not developmentally toxic via the inhalation route of exposure. Inhalation of saturated vapors of 1-hexanol (3500 mg/m^3, 7 hr/day, GD 1-19) resulted in no significant signs of maternal or fetal toxicity. The NOAEL for both maternal and fetal effects for this study was the limit dose of 3500 mg/m^3.

Another study evaluated the developmental toxicity of three structurally related alcohols, 1-octanol, 1-nonanol, and 1-decanol following inhalation. Sprague-Dawley rats were exposed to saturated vapors of 1-octanol (400 mg/m^3), 1-nonanol (150 mg/m^3), and 1-decanol (100 mg/m^3) for 7 hours per day during days 1-19 of gestation. No significant effects, including no changes in maternal weight gain, feed consumption, or water intake were observed between the control and any of the treated groups. In addition, no fetal toxicity was observed, as indicated by fetal body weight, sex ratio, and the number of resorptions. The NOAEL for both maternal and fetal effects for each test substance was the saturated vapor concentration: 1-octanol (400 mg/m^3), 1-nonanol (150 mg/m^3), and 1-decanol (100 mg/m^3).

Collectively, the weight of evidence demonstrates that Alkyl Alcohols C6-C13 have a low order or maternal toxicity and do not induce signs of developmental toxicity until maternal toxicity is observed. Hence, these materials are not selective developmental toxicants. In addition, the maternal and fetal NOAELs for oral exposure to different members of the category are consistent. Furthermore, the NOAELs for inhalation reflect the maximum achievable vapor concentration. Since these materials are not selective toxicants and display a consistent, low order of developmental toxicity they will not undergo further testing for developmental toxicity.

Reproductive Toxicity

The available reproductive toxicity studies and repeat-dose studies prove adequate to support a screening-level hazard assessment for the reproductive toxicity potential of Alkyl Alcohols C6 - C13. Developmental toxicity studies conducted by the oral route of exposure on Isooctyl alcohol, Isononyl alcohol, Isodecanol, and Undecyl alcohol, produced consistent results and demonstrated that these materials do not affect reproductive parameters. Although a slight increase in resporptions was observed in several studies, this only occurred in the highest dose group and in the presence of overt maternal toxicity. Furthermore, inhalation exposure to saturated vapors of 1-hexanol, 1-octanol, 1-nonanol, and 1-decanol did not induce any significant changes in reproductive parameters. In the subacute studies of isooctyl alcohol and isononyl alcohol, no changes in testicular weight were observed. These data support the conclusion that the Alkyl Alcohols C6-C13 are not selective reproductive toxicants. According to the OECD SIDS Guidelines, adequate developmental toxicology data coupled with subchronic toxicity data that shows no effects on reproductive organs fulfills the requirement for an assessment of reproductive toxicity potential.

D. Aquatic Toxicity

The alkyl alcohol products ranging from hexanol, branched and linear, to C11-C14 iso, C13 rich, have been shown to produce an expected increasing level of acute toxicity to freshwater fish and invertebrates. This is based on data from the literature that are used to read across to selected alcohol products in this test plan, company data specifically for products in this category, as well as results of computer modeling using ECOSAR for selected chemical components of products in this category [ECOSAR is an aquatic toxicity modeling program and is a subroutine contained in EPIWIN model]. Although there are insufficient data to confirm that a similar pattern of alga toxicity exists, based on the fish and invertebrate data, a similar increasing level of toxicity is expected from the lower to higher molecular weight products. Proposed testing will develop the data needed to confirm this expectation. Based on the existing data, products in the Alkyl Alcohols C6 - C13 Category demonstrate a moderate to high degree of aquatic toxicity from the low to high molecular weight products, respectively.

Fish Acute Toxicity

TEST	Hexanol, branched and linear	Alcohols C6-8, branched	Alcohols C7-9, branched	Alcohols C8-10 iso, C9 rich	Alcohols C9-11 iso, C10 rich	Alcohols C11-14 iso, C12 rich,	Alcohols C11-14 iso, C13 rich
FISH ACUTE TOXICITY (96-hour)	LC_{50}= 97.7 mg/L (Brooke, 1984)	LC_{50}= 34.5 mg/L (Geiger, 1986)	LC_{50}= 14.0 mg/L (Geiger, 1988)	LC_{50}= 10.1 mg/L (EBSI, 1996a)	LC_{50}= 3.1 mg/L (EBSI, 1996b)	LC_{50}= 1.2 mg/L (EBSI, 1997c)	LC_{50}= 0.42 mg/L (EBSI, 1998a)

RA read across

Acute experimental toxicity test results are reported for rainbow trout (*Oncorhynchus mykiss*) and fathead minnow (*Pimephales promelas*). Hexanol, branched and linear, through C11-14 iso, C13 rich, alkyl alcohol products have the potential to cause acute toxicity (96-hour LC_{50}) within a range of approximately 98 to 0.4 mg/L.

Invertebrate Acute Toxicity

TEST	Hexanol, branched and linear	Alcohols C6-8, branched	Alcohols C7-9, branched	Alcohols C8-10 iso, C9 rich	Alcohols C9-11 iso, C10 rich	Alcohols C11-14 iso, C12 rich,	Alcohols C11-14 iso, C13 rich
DAPHNID ACUTE TOXICITY (48-hour)	RA	LC_{50}= 63 mg/L (Canton, 1978)	LL_{50}= 31.8 mg/L (Union Carbide, 1980)	LC_{50}= 4.9 mg/L (EBSI, 1996c)	RA	LC_{50}= 0.81 mg/L (EBSI, 1997d)	LC_{50}= 0.71 mg/L (EBSI, 1987)
DAPHNID ACUTE TOXICITY (48-hour)**	C6 OH LC_{50}= 137 mg/L (ECOSAR, 1999)	C7 OH LC_{50}= 56 mg/L (ECOSAR, 1999)	C8 OH LC_{50}= 22 mg/L (ECOSAR, 1999)				

** ECOSAR modeled data
OH alcohol

Experimental and modeled data show that these products have the potential to cause acute toxicity (48-hour EL_{50} or EC_{50}) within a range of approximately 137 to 0.7 mg/L. Acute experimental toxicity test results for five alkyl alcohol products are reported for a Daphnid (*Daphnia magna*). Experimental data for the hexanol, branched and linear, product are not available, but results from ECOSAR (1999), an aquatic toxicity computer model, can be used to adequately characterize the aquatic toxicity of this product.

Results of computer modeling for a C7 and C8 branched alcohol are consistent with the experimental data used to characterize the toxicity of the C6-8 and C7-9 branched alcohol products. This suggests that the ECOSAR model is sufficiently robust to accurately calculate the toxicity of this range of chemicals. Therefore, the modeled value for a C6 alcohol is expected to be consistent with an experimental value for a hexanol, branched and linear, product and will be used to characterize the range of Daphnid acute toxicity for the Alkyl Alcohol C6 - C13 Category. The Kow values used to

calculate the toxicity values for the C6, C7, and C8 alcohols were 1,75, 2,24, and 2,73, respectively. These values were calculated using the EPIWIN (1999) computer model.

Alga Toxicity

TEST	Hexanol, branched and linear	Alcohols C6-8, branched	Alcohols C7-9, branched	Alcohols C8-10 iso, C9 rich	Alcohols C9-11 iso, C10 rich	Alcohols C11-14 iso, C12 rich,	Alcohols C11-14 iso, C13 rich
ALGA TOXICITY (96-hour)	TESTING PROPOSED	RA	RA	LC_{50}= 8.5 mg/L (Bringmann, 1980)	RA	RA	TESTING PROPOSED

RA read across

An acute experimental toxicity threshold value is reported for the freshwater alga (*Scenendesmus quadricauda*) and used as read across data to the C8-10 iso, C9 rich alkyl alcohol product. This result suggests that the C9-11, C10 rich, alkyl alcohol has the potential to cause acute toxicity (based upon cell growth) at a concentration of above 8.5 mg/L. However, this study is not sufficient to adequately characterize the toxicity of products in this category to an alga.

ExxonMobil Chemical believes that the alga toxicity of the Alkyl Alcohols C6-C13 Category should be characterized by developing data for the hexanol, branched and linear, and the C11-14 iso, C13 rich, alkyl alcohol products to adequately characterize this endpoint. Data from fish and invertebrate acute toxicity studies show a consistent trend of increasing toxicity as carbon number and molecular weight increases. Acute toxicity to an alga is expected to follow the same trend and the proposed testing should appropriately define that range of toxicity. The one experimental value identified above will provide an intermediate toxicity value, which in conjunction with results from the proposed testing should provide adequate data to demonstrate an increasing range of alga toxicity for products in this category.

E. Environmental Fate

Biodegradation data are available for four alkyl alcohol products. They show that these alcohol products have the potential to biodegrade to a great extent within a standard 28-day test duration, which suggests that products in this category will not persist in the environment.

Although there is some information on photodegradation and fugacity, a complete data set to adequately characterize the alkyl alcohol products does not exist. Chemical equilibrium models are used to calculate fugacity, which describes the potential of a chemical to partition in the environment. These data can only be calculated. Preliminary information for selected component chemicals of products in the Alkyl Alcohol C6 - C13 Category suggests that these products are expected to partition primarily to water and soil. However, their fate in air is of environmental interest (this is discussed below under photodegradation). In addition, the majority of the component chemicals in these products have relatively low K_{ow} values, which suggests that they will

not tend to partition to suspended organic matter in air and precipitate to aquatic and terrestrial environmental compartments to a significant extent.

Biodegradation

TEST	Hexanol, branched and linear	Alcohols C6-8, branched	Alcohols C7-9, branched	Alcohols C8-10 iso, C9 rich	Alcohols C9-11 iso, C10 rich	Alcohols C11-14 iso, C12 rich,	Alcohols C11-14 iso, C13 rich
28-Day Aerobic Biodegra-dation Test	RA	RA	82% (EBSI, 1996d)	RA	71.1% (EBSI, 1997e)	59% (EBSI, 1997f)	58% (EBSI, 1998b)

RA read across

C7-C9 branched, and C9-C11 branched alkyl alcohol products have been shown to biodegrade rapidly using a 28-day standard biodegradation test procedure. In comparison, C11-C14 iso, C12 rich, and C11-C14 iso, C13 rich alkyl alcohol products biodegrade to slightly lower but significant extents, which suggests that although they are not expected to degrade at rates equivalent to the lighter alkyl alcohol products, they will not persist in the environment.

Upon review of the available information, sufficient quality data were identified to accurately characterize the biodegradability of the products in this category. The data show that these products can biodegrade to an extent ranging from approximately 58 to 82% after 28 days. These data were developed using non acclimated inocula obtained from wastewater treatment plants. The tests used closed systems, which is required when assessing the biodegradability of potentially volatile materials like those in this category. The test systems were continuously stirred, which is also recommended when evaluating mixtures containing several chemicals, some of which may have minimal water-solubility.

Photodegradation – Photolysis (Direct)

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may undergo a transformation. Simple chemical structures can be examined to determine whether a chemical has the potential for direct photolysis in water. First order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline (Zepp, 1977). UV light absorption of the chemical components in this category will be evaluated to identify those having the potential to degrade in solution. For those compounds with a potential for direct photolysis in water, first order reaction rates will be calculated. A technical document will be prepared that summarizes the results of information developed for this endpoint.

Photodegradation – Atmospheric Oxidation (Indirect)

Photodegradation can be measured (US EPA, 1999a) (EPA identifies OECD test guideline 113 as a test method) or estimated using models accepted by the EPA (US EPA, 1999b). An estimation method accepted by the EPA includes the calculation of atmospheric oxidation potential (AOP).

Atmospheric oxidation as a result of hydroxyl radical (OH-) attack is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model. Alkyl alcohol products, such as those in this category, have the potential to volatilize to air. Preliminary data suggest that the potential ranges from moderate to low for the chemical components of products in this category. In air, those chemicals with a higher potential to volatilize may undergo reaction with photosensitized oxygen in the form of ozone and hydroxyl radicals.

The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPIWIN, 1999) is used by OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH- reaction rate constant, a 12-hr day, and a given OH- concentration. This calculation will be performed for the representative chemical components in this category and summarized in robust summaries for this group of products.

Stability in Water (Hydrolysis)

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). Stability in water can be measured (US EPA, 1999a) (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA (US EPA, 1999b).

All of the chemical structures included in this category are alkyl alcohols. As such they are not expected to hydrolyze at a measurable rate. A technical document will be prepared that discusses the nature of the chemical bonds present and the potential reactivity of this class of chemicals with water. This information will be summarized in robust summaries for this group of products.

Chemical Transport and Distribution In The Environment (Fugacity Modeling)

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model (Mackay, 1996). EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data* (US EPA, 1999a), which was prepared as guidance for the HPV Program.

In its document, EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments (air, soil, water, suspended sediment, sediment, biota) within a unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. This model will be used to calculate distribution values for representative chemical components identified in products in this category. A computer model, EPIWIN – version 3.02 (EPIWIN, 1999), will be used to calculate the properties needed to run the Level I EQC model. This information will be summarized in robust summaries for this group of products.

IV. TEST PLAN SUMMARY

ExxonMobil Chemical believes that the Alkyl Alcohols C6 - C13 Category of products should be further examined in the following manner:

- Calculate physicochemical data as described in the EPA document titled, *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program* for selected chemical components of the alkyl alcohol products in this category. Provide measured data for selected products where readily available.
- Prepare a technical discussion on the potential of alkyl alcohol products in this category to photodegrade. Calculate AOP values for selected chemical components of alkyl alcohol products in this category.
- Prepare a technical discussion on the potential of alkyl alcohol products in this category to hydrolyze.
- Calculate fugacity data for selected chemical components of alkyl alcohol products in this category.
- Conduct two acute algal toxicity assays, one with a hexanol, branched and linear, and a second with an alcohol C11-C14, C13 rich, products.
- Conduct one mouse micronucleus assay with a alkyl alcohol C6 product.

ExxonMobil Chemical Company believes the thorough evaluation of the strategic anchor studies, the development of selected information and data, and the overall robustness of the final screening data set for an Alkyl Alcohols C6 -C13 Category complies with the objectives of the HPV Chemical Challenge program.

REFERENCES

Brooke, L.T., D.J. Call, Geiger, D.L. and C.E. Northcott, (1984). "Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*). Vol. 1. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, Superior, WI. Pp. 179-180.

Bringmann, G. and R. Kühn. (1980). "Comparison of the Toxicity Thresholds of Water Pollutants to Bacteria, Algae, and Protozoa in the Cell Multiplication Inhibition Test." Water Research **14**: 231-241.

Canton, J.H., and D.M.M. Adema. (1978). "Reproducibility of Short-term and Reproduction Toxicity Experiments with *Daphnia magna* and Comparison of the Sensitivity of *Daphnia magna* with *Daphnia pulex* and *Daphnia cucullata* in Short-term Experiments." Hydrobiologica **59(2)**: 135-140.

EPIWIN, (1999). Estimation Program Interface for Windows, version 3.02. Syracuse Research Corporation, Syracuse, NY, USA.

Esso Research and Engineering (1960a). Acute Oral Toxicity of Isodecanol in Rats. Unpublished report.

Esso Research and Engineering (1960b). Acute Dermal Toxicity of Isodecanol in Rabbits. Unpublished report.

Esso Research and Engineering Company (1961a). Repeat Dermal Application of Hexyl Alcohol. Unpublished report.

Esso Research and Engineering Company (1961b). Repeat Dermal Application of Isooctyl Alcohol. Unpublished report.

Esso Research and Engineering (1968a), Histopathological Evaluation. Supplement to Repeated Dermal Application Report. Unpublished report.

Esso Research and Engineering (1968b). Acute Oral Toxicity of Isononyl Alcohol in Rats. Unpublished report.

Esso Research and Engineering (1968c). Acute Dermal Toxicity of Isononyl Alcohol in Rabbits. Unpublished report.

Esso Research and Engineering (1979a). Acute Oral Toxicity Study of Isoheptyl Alcohol in Rats. Unpublished report.

Esso Research and Engineering (1979b). Acute Dermal Toxicity of Isoheptyl Alcohol in Rabbits. Unpublished report.

Esso Research and Engineering (1980). Acute Inhalation Toxicity of Isoheptyl Alcohol in Rats, Mice, and Guinea Pigs. Unpublished report.

European Chemicals Bureau (ECB) (2000a). IUCLID Data Set, Hexan-1-ol (CAS#: 111-27-3).

European Chemicals Bureau (ECB) (2000b). IUCLID Data Set, 2-ethylhexan-1-ol (CAS#: 104-76-7).

European Chemicals Bureau (ECB) (2000c). IUCLID Data Set, Dodecan-1-ol (CAS#: 112-53-8).

Exxon Biomedical Sciences, Inc. (EBSI) (1987). A Static Acute *Daphnia* Toxicity Test. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1994a). Developmental Toxicity Study of Isooctyl Alcohol in Rats. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI). 1994b. East Millstone, NJ, USA. Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay with C7-C9 Branched Alkyl Acetate Ester. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI), 1994c. East Millstone, NJ, USA. Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay with C11-C14 Branched Alkyl Acetate Ester. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI). 1994d. East Millstone, NJ, USA. In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method with C7-C9 Branched Alkyl Acetate Ester. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI), 1994e. East Millstone, NJ, USA. In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method with C11-C14 Branched Alkyl Acetate Ester. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI), 1995a. East Millstone, NJ, USA. Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay with C6 Branched and Linear Alkyl Acetate Ester. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI), 1995b. East Millstone, NJ, USA. In Vitro Chromosomal Aberration Assay in CHO Cells with C6 Branched and Linear Alkyl Acetate Ester. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1996a). Fish Acute Toxicity Test. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1996b). Fish Acute Toxicity Test. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1996c). Acute Toxicity for *Daphnia*. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1996d). Ready Biodegradability: OECD 301F Manometric Respirometry Test. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1997c). Fish Acute Toxicity Test. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1997d). Acute Toxicity for *Daphnia*. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1997e). Ready Biodegradability: OECD 301F Manometric Respirometry Test. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1997f). Ready Biodegradability: OECD 301F Manometric Respirometry Test. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1998a). Fish Acute Toxicity Test. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1998b). Ready Biodegradability: OECD 301F Manometric Respirometry Test. Unpublished report.

Exxon Biomedical Sciences, Inc. (EBSI) (1998c). N-Octanol/Water Partition Coefficient. Unpublished report.

Geiger, D.L., D.J. Call, and L.T. Brooke. (1988). "Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*). Vol. 4. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, Superior, WI. Pp. 183-184.

Geiger, D.L., S.H. Poirier, L.T. Brooke, and D.J. Call. (1986). "Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*). Vol. 3. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, Superior, WI. Pp. 181-182.

Hazleton Labs (1960) "Acute oral, acute dermal, and acute inhalation toxicity of Hexyl alcohol, Isoheptyl alcohol, and Isooctyl Alcohol." Unpublished report.

Hazleton Laboratories Incorporated (HLI), (1963) Falls Church, VA, USA. Unpublished report.

Klimisch, H. J., M. Andreae, and U. Tillmann, (1997). A Systematic Approach for Evaluating the Quality of Experimental Toxicological and Ecotoxicological Data. Regulatory Toxicology and Pharmacology. 25:1-5.

Lington, A.W. and Bevan, C., (1994). Patty's Industrial Hygiene and Toxicology, Fourth Edition, John Wiley & Sons, Inc, Chapter Thirty, "Alcohols," pp. 2585-2710.

Mackay, D., A. Di Guardo, S. Paterson, and C. E. Cowan, (1996). Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15:1627-1637.

Mann, A.H., (1987). An assessment of the likely metabolic fate of some isomers of hexyl acetate. The Robins Institute of Industrial & Environmental Safety, University of Surrey, Guildford Surrey, U.K.

Monick, J.A., (1968). Alcohols. Their Chemistry, Properties and Manufacture. Reinhold Book Corporation, NY.

Neely, W. B., (1985). Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

Nelson, B.K., Brightwell, W.W., Khan, A., Krieg, E.F., Jr., Hoberman, A.M., (1989). "Developmental toxicology evaluation of 1-pentanol, 1-hexanol, and 2-ethyl-1-hexanol administered by inhalation to rats." Journal of the American College of Toxicology **8(2)**: 405-410. NIOSH, Division of biomedical and behavioral sciences.

Nelson, B.K., Brightwell, W.W., Khan, A., Krieg, E.F., Jr., Hoberman, A.M., (1990). "Developmental toxicology assessment of 1-Octanol, 1-Nonanol, and 1-Decanol administered by inhalation to rats." Journal of the American College of Toxicology **9(1)**: 93-97.

RCC Research and Consulting Co. (1988a) "Acute oral toxicity study with Isooctyl Alcohol in rats." Unpublished report.

RCC Research and Consulting Co., (1988b) "Acute Oral Toxicity Study Isododecanol in Rats." Unpublished report.

RCC Research and Consulting Co., (1988c) "Acute Oral Toxicity of Tridecyl Alcohol Study in Rats." Unpublished report.

Rhodes, C., Soames, T., Stonard, M.D., Simpson, M.G., Vernall, A.J., Elcombe, C.R, (1984). "The absence of testicular atrophy and in vivo and in vitro effects on hepatocyte morphology and peroxisomal enzyme activities in male rats following the administration of several alkanols," Toxicology Letters 21: 103-109.

Shimizu, H., Suzuki, Y., Takemura, N., Goto, S., Matsushita, H., (1985) "The Results of Microbial Mutation Test for Forty-Three Industrial Chemicals," *Japanese Journal of Industrial Health*, 27: 400-419.

US EPA TSCA 8(e) Submission: (1989a) Study of the Prenatal Toxicity of Isononylalcohol 1 and Isononylalcohol 2 in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000247.

US EPA TSCA 8(e) Submission: (1989b) Study of the Prenatal Toxicity of Isodecanol, 2-Ethylhexanol, and 711 Alcohol (T.C.) in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000245.

Union Carbide Corp. (1980). "The Acute Toxicity of MRD-80-4 to the Water Flea (*Daphnia magna* Straus)." Unpublished report.

US EPA, (1999a). Determining the Adequacy of Existing Data. OPPT, EPA., Washington, DC, USA.

US EPA, (1999b). The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program. OPPT, EPA, Washington, DC, USA.

Wislocki, P.G., Miwa, G.T., and Lu, A.Y.H., (1980). Reactions Catalyzed by the Cytochrome P-450 System. Enzymatic Basis of Detoxification. Vol. I (ed. W.B.Jakoby), Academic Press, New York, NY.

Zepp, R. G., and D. M. Cline, (1977). Rates of Direct Photolysis in the Aqueous Environment. Environ. Sci. Technol. 11:359.366.

Table 3. Assessment Plan for the Alkyl Alcohols C6-C13 Category Under the Program. (Robust summaries for existing studies are submitted separately.)

Stream Description	Human Health Effects						Ecotoxicity			Environmental Fate				
	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Develop-mental	Reproduction	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.[1]	Photo-deg.	Hydro-lysis	Fugacity	Biodeg.
Hexyl alcohol	A	A	T	A	A	A	A	CM	T	CM	TD	TD	CM	RA
Alkyl alcohol C6-8, branched	A	RA	RA	RA	RA	RA	A	A	RA	CM	TD	TD	CM	RA
Alkyl alcohol C7-9, branched	A	A	A	A	A	A	A	A	RA	CM	TD	TD	CM	A
Alkyl alcohol C8-10, branched	A	RA	RA	A	A	A	A	A	A	CM	TD	TD	CM	RA
Alkyl alcohol C9-11, branched	A	RA	RA	RA	A	A	A	RA	RA	CM	TD	TD	CM	A
Alkyl alcohol C11-14, branched	A	A	A	A	RA	RA	A	A	T	CM	TD	TD	CM	A

1 Measured data for selected physicochemical endpoints will be identified in conjunction with calculated data to characterize this category.

A Adequate existing data available
CM Computer Modeling proposed
NA Not Applicable
TD Technical Discussion proposed
T Testing proposed
RA Read Across (see Sec. III.B)

AR201-13590B

Alkyl Alcohols C6-C13 Category

Robust Summaries
Mammalian Effects

RECEIVED
OPPT NCIC
02 FEB -6 AM 9:57

Prepared by:

ExxonMobil Chemical Company

November 15, 2001

(Revised February 5, 2002)

Table of Contents

CAS # 68526-79-4; Hexanol, branched and linear
- Acute Oral
- Acute Dermal
- Acute Inhalation
- Repeat Dose - Dermal
- Developmental Toxicity (1-hexanol)

CAS # 70914-20-4; Alcohols C6-8, branched
- Acute Oral
- Acute Dermal
- Acute Inhalation

CAS #68526-83-0; Alcohols C7-9, branched
- Acute Oral
- Acute Dermal
- Acute Inhalation
- Genetic Toxicity - Ames Assay (2-ethyl-1-hexanol)
- Repeat Dose
- Repeat Dose - Dermal
- Developmental Toxicity (1-octanol)
- Developmental Toxicity

CAS # 68526-84-1; Alcohols C8-10 iso, C9 rich
- Acute Oral
- Acute Dermal
- Repeat Dose
- Developmental Toxicity (Isononyl alcohol 1)
- Developmental Toxicity (Isononyl alcohol 2)
- Developmental Toxicity (1-nonanol)

CAS #68526-85-2; Alcohols C9-11 iso, C10 rich
- Acute Oral
- Acute Dermal
- Developmental Toxicity (Isodecanol)
- Developmental Toxicity (1-decanol)
- Developmental Toxicity (C7-9-11 Alcohol)

CAS #68526-86-3; Alcohols C11-14 iso, C13 rich
- Acute Oral
- Genetic Toxicity - Ames Assay (1-dodecanol)

Acute Toxicity

Test Substance	Hexanol, branched and linear
CAS No.	68526-79-4
Method/Guideline	Other
Type of Study	Oral LD_{50}
GLP	Pre-GLP
Year	1960
Species/strain	Rats/Sprague-Dawley
Sex	Males
No. of animals/sex/dose	5 rats/dose
Route of administration	Gastric Intubation
Vehicle	None
Frequency of Treatment	Single exposure
Dose/Concentration Levels	26, 82, 259, 820, 2591, 8200 mg/kg
Control group and Treatment	None
Remarks on Test Conditions	After a three to four hour fasting period, groups of 5 rats received the test material at dose levels of 26, 82, 259, 820, 2591, and 8200 mg/kg of body weight. The results were converted to weight units by means of the specific gravity. Observations for signs of toxicity were made immediately and at one and 24 hours after compound administration and daily for a period of 7days. Gross necropsy examinations were performed on all animals that died or were killed.
Results	LD_{50}= 3670 mg/kg
Remarks	None of the animals died in the 26, 82, 259, and 820 mg/kg dose groups. One of the animals in the 2591 mg/kg group died within 24 hours of dosing. All animals in the 8200 mg/kg group died within 4 hours following dose administration. Treatment resulted in depression (i.e. inactivity, depressed righting reflexes, ataxia) and labored respiration. These signs had an early onset and recovery was complete by the second day after dosing. Gross necropsy on the animals that died showed congested kidneys. Also, animals that died during the first hour after administration showed evidence of gastrointestinal irritation.
Conclusions	Under the conditions of this study, Hexanol, branched and linear has a low order of acute oral toxicity in rats.
Data Quality	1 - Valid without restrictions
Reference	Hazleton Laboratories (1960). Acute oral administration, acute dermal application, and acute inhalation exposure. Unpublished report.
Date last changed	September, 2000

Acute Toxicity

Test Substance	Hexanol, branched and linear
CAS No.	68526-79-4
Method/Guideline	Other
Type of Study	Acute dermal toxicity
GLP	Pre-GLP
Year	1960
Species/strain	Albino Rabbits
Sex	Males and Females
No. of animals/sex/dose	2 rabbits/sex/dose
Route of administration	Dermal Application
Vehicle	None
Frequency of Treatment	Single exposure
Dose/Concentration Levels	82, 259, 820, and 2600 mg/kg
Control group and Treatment	None
Remarks on Test Conditions	A single dermal application of the test material was made to four groups of four rabbits at doses of 82, 259, 820, and 2600 mg/kg. The results were converted to weight units by means of the specific gravity. The test material was applied to intact abdominal skin and covered with an occlusive covering for 24 hours. Observations for signs of toxicity were made at one, four and 24 hours after compound administration and thereafter for a total of 7 days. Gross necropsies were performed on all animals at the end of the observation period.
Results	LD_{50} > 2600 mg/kg
Remarks	There were no mortalities at any dosage level tested. The LD_{50} in albino rabbits is greater than the highest dose tested (approx. 2.6 g/kg body weight). Signs of toxicity included labored respiration and central nervous system depression. All animals recovered within 4-48 hours after the exposure period began. Moderate erythema and edema were observed.
Conclusions	Under conditions of this study, Hexanol, branched and linear has a low order of acute dermal toxicity in rabbits.
Data Quality	2 - Valid with restrictions.
Reference	Hazleton Laboratories (1960). Acute oral administration, acute dermal application, and acute inhalation exposure. Unpublished report.
Date last changed	September, 2000

Acute Toxicity

Test Substance	Hexanol, branched and linear
CAS No.	68526-79-4
Method/Guideline	Other
Type of Study	Inhalation LC_{50}
GLP	Pre-GLP
Year	1960
Species/strain	Rats/Wistar, Mice/Swiss, Guinea Pigs/English short hair
Sex	Males
No. of animals/sex/dose	10/species
Route of administration	Inhalation
Vehicle	NA
Frequency of Treatment	Single 6 hour exposure
Dose/Concentration Levels	1060 ppm
Control group and Treatment	None
Remarks on Test Conditions	Rats, mice, and guinea pigs received a single, 6-hour exposure to the test material in air. Exposures were at atmospheres nearly saturated with vapors of the alcohol (1060 ppm). The exposure was conducted in a 500-liter stainless steel inhalation chamber equipped at the inlet with a device for generating a near-saturated vapor of the test material. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml. Of the test material. Air flow through each bubbler was 18 liters/minute, so the total flow through the chamber was 36 liters/min. Actual chamber concentration was not measured during the exposure. The theoretical chamber concentration was calculated to be 1060 ppm based upon the amount of test material that vaporized and the rate of air flow. During exposure, all animals were observed for gross signs of toxicity at 30-minute intervals. Gross necropsies were performed on animals 24 hours after exposure.
Results	LC_{50} > 1060 ppm for rats, mice and guinea pigs.
Remarks	No deaths were seen during or after the exposure period. Thirty minutes after exposure, slow, deep respiration was observed in all three species. After 90 minutes of exposure, all three species exhibited gasping, labored respiration, lacrimation and nasal discharge. These signs persisted until the termination of exposure. Gross necropsy results indicate that the test material produced slight lung congestion in all animals. All other tissues and organs were unremarkable.
Conclusions	Under the conditions of this study, Hexanol, branched and linear has a low order of acute inhalation toxicity in rats, mice and guinea pigs.
Data Quality	2 - Valid with restrictions - No analysis of exposure atmosphere.
Reference	Hazleton Laboratories (1960). Acute oral administration, acute dermal application, and acute inhalation exposure. Unpublished report.
Date last changed	September, 2000

Repeat Dose Toxicity

Test Substance	Hexanol, branched and linear
CAS No.	68526-79-4
Method/Guideline	Other
Test Type	Repeated Dermal Application
GLP	Pre-GLP
Year	1961
Species/strain	Albino Rabbits
Route of administration	Dermal
Duration of test	12 days
Number of animals	8 (2/sex/dose)
Dose/Conc. Levels	0.4 g/kg and 2.0 g/kg
Sex	Males and Females
Frequency of treatment	Single daily treatment for 10 days
Control group and treatment	Isopropyl alcohol
Remarks on Test Conditions	Undiluted control and test materials were applied to intact skin of the animals. Materials were applied once daily for a total of ten applications with a one-day rest period between the third and fourth and eighth and ninth applications. The exposed skin area of each animal was approximately 10% of the total body surface at the 0.4 g/kg dosage level and approximately 40% of the total body surface at the 2.0 g/kg dosage level. After the first application, exposed skin was covered by rubber dental damming. In subsequent applications, loose gauze and adhesive tape were used to cover the exposed area since the authors felt that the damming itself may have induced some irritation. Each exposure period lasted approximately 18-24 hours. Animals were observed daily throughout the study and body weights were recorded prior to each application and at study termination. Clinical hematology and urinalysis were performed at the beginning of the study and 24 hours after the final application of test material. Animals were sacrificed 48 hours after the tenth application and brain, liver, kidney, and blood samples were taken. In addition, samples of brain, thyroid, lung, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved.
Results	NOAEL for systemic toxicity = 2.0 g/kg
Remarks	There was no evidence of systemic toxicity at either dose of the test substance. Histopathological findings were unremarkable. Repeated application of the test material to the skin of albino rabbits at both dose levels produced moderate to marked degree of irritation. A slight to marked degree of edema was observed in two low-dose animals and three high-dose animals following one or more of the first three applications. Also, the exposed skin of two high-dose animals showed necrosis.
Conclusions	Under the conditions of this study, Hexanol, branched and linear can produce moderate skin irritation following repeated dermal exposures. However, the test material did not produce any evidence of systemic toxicity under the conditions of this study.
Data Quality	2 - Valid with restrictions.
Reference:	Esso Research and Engineering Company (1961). Unpublished Report.
Date last changed	September, 2000

Developmental Toxicity

Test Substance	1-Hexanol
CAS No.	--
Method/Guideline	Other
Type of Study	Developmental Toxicity
GLP	Not specified
Year	1989
Species/strain	Rats/Sprague-Dawley
Sex	Females
No. of animals/sex/dose	15 dams/treatment
Route of administration	Inhalation
Frequency of treatment	7 hrs/day; Gestation days 1-19
Dose/Concentration Levels	3500 mg/m^3 (Saturated vapors)
Control group and treatment	15 sham-exposed rats
Statistical methods	MANOVA, ANOVA, Kruskal-Wallis test
Remarks on Test Conditions	Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the test substance was ≥ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heat compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 3500 mg/m^3. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by CO_2 asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects.
Results	NOAEL > 3500 mg/m^3
Remarks	The test substance was administered by inhalation to reflect the route of exposure found in industry. However, due to the low volatility of the alcohols, concentrations sufficient to induce maternal toxicity could not be achieved. There were no significant fetal malformations associated with inhalation of 1-hexanol by the dam. There was a slight but statistically significant increase in resorptions (1.3 vs. 0.4 per litter for controls). However, this resorption mean was still in the range seen in historical controls.

Conclusions	Inhalation of saturated vapors of 1-hexanol is not maternally toxic or teratogenic in rats.
Data Quality	2 - Reliable with restrictions.
Reference	B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology evaluation of 1-pentanol, 1-hexanol, and 2-ethyl-1-hexanol administered by inhalation to rats." (1989) Journal of the American College of Toxicology **8(2)**: 405-410. NIOSH, Division of Biomedical and Behavioral Sciences
Date last changed	13-Sep-00

Acute Toxicity

Test Substance	Alcohols, C6-8 branched
CAS No.	70914-20-4
Method/Guideline	Other
Type of Study	Acute oral toxicity
GLP	Not specified
Year	1979
Species/strain	Rats/Sprague/Dawley
Sex	Males
No. of animals	5/dose
Route of administration	Oral Intubation
Vehicle	None
Frequency of Treatment	Single Exposure
Dose/Concentration Levels	1.0, 1.47, 2.15, 3.16, 4.64, 6.81 and 10.0 g/kg
Control group and Treatment	None
Remarks on Test Conditions	Animals were fasted for approximately 18 hours prior to dosing. The undiluted test material was administered by oral intubation at doses of 1.0, 1.47, 2.15, 3.16, 4.64, 6.81 and 10.0 g/kg (5 rats/dose). Animals were observed for signs of toxicity at 1, 2, and 4 hours after dosing and daily thereafter for fourteen days.
Results	LD_{50} = 3.9 g/kg
Remarks	All animals in the 6.81 and 10.00 g/kg groups died. Two of the five animals in the 4.64 g/kg group died and 1 animal each in the 1.00, 2.15, and 3.15 g/kg groups died. No animals in the 1.47 g/kg group died. Except for one animal in the 2.15 g/kg group, all animals that died did so within three days of dosing. Signs of toxicity observed included respiratory rate decreases, fecal staining, decreased motor activity and hypothermia.
Conclusions	Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute oral toxicity.
Data Quality	2 - Valid with restrictions - only one sex tested.
Reference	"Acute Oral Toxicity Study in Rats," Esso Research and Engineering (1979). Unpublished report.
Date last changed	September, 2000

Acute Toxicity

Test Substance	Alcohols, C6-8 branched
CAS No.	70914-20-4
Method/Guideline	Other
Type of Study	Acute dermal toxicity
GLP	Not specified
Year	1979
Species/strain	Albino Rabbits/New Zealand White
Sex	Males and Females
No. of animals/sex/dose	2 rabbits/sex/dose
Route of administration	Dermal
Vehicle	None
Frequency of Treatment	Single dose
Dose/Concentration Levels	50, 200, 794 and 3,160 mg/kg
Control group and Treatment	None
Remarks on Test Conditions	Doses of 50, 200, 794 and 3160 mg/kg were administered to sixteen rabbits (two/sex/dose level). The undiluted test material was applied to intact skin and the animal was then wrapped in an impervious plastic sleeve. Following approximately 24 hours of exposure, the wrappings were removed and the test site was wiped free of excess test material. After 30 minutes, dermal observations were made. Observations were recorded at 1, 2 and 4 hours after dosing and daily thereafter for 14 days.
Results	LD_{50} > 3,160 mg/kg of body weight.
Remarks	There were no deaths at any dose level in either sex. All animals at the 50 mg/kg level exhibited very slight erythema and no edema. Well-defined erythema without edema was observed in animals at 200 and 794 mg/kg dose levels. At the 3160 mg/kg dose level one animal exhibited moderate to severe erythema and three animals exhibited areas of necrosis. Necropsy examinations did not reveal any significant abnormalities. Dark red foci were observed in the lungs of males (50mg/kg) and females (3,160 mg/kg), however this effect was not dose-related. Dark red foci of the adrenals were observed in males and females at 200, 794, and 3,160 mg/kg.
Conclusions	Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute dermal toxicity in rats.
Data Quality	2 - Valid with restrictions - GLP not specified.
Reference	Esso Research and Engineering (1979). Unpublished report.
Date last changed	September, 2000

Acute Toxicity

Test Substance	Alcohols, C6-8 branched
CAS No.	70914-20-4
Method/Guideline	Other
Type of Study	Acute inhalation toxicity
GLP	Not specified
Year	1979
Species/strain	Rats/Sprague-Dawley, Mice/Swiss albino, Guinea pigs/Hartley
Sex	Males and Females
No. of animals/sex/dose	5/sex/dose
Route of administration	Inhalation
Vehicle	NA
Frequency of Treatment	Single, 6 hour exposure
Dose/Concentration Levels	0, 152 ppm
Remarks on Test Conditions	Animals (5/sex/dose) were held for a minimum equilibration period of 12 days. Animals were exposed to 152 ppm of the test material for six hours. To generate vapors, room air was drawn through the test material at a flow rate of 103 l/min. The resulting maximum attainable vapors were passed through a Kjeldahl trap and flask prior to entering the glass exposure chamber containing the test animals. Weight loss was determined following exposure and was taken to be equal to the amount of test material delivered during exposure. The weight loss was divided by the total volume of air passed through the chamber to give the nominal concentration. All three species were exposed in the same chamber. For each species, a control group was also sham-exposed to room air. The animals were observed for abnormalities prior to exposure, at 15-minute intervals during the first hour of exposure and then hourly for the remainder of exposure. Subsequent evaluations were made for a total of 14 days. After fourteen days, gross necropsy was performed.
Results	LC_{50} > 152 ppm
Remarks	No abnormalities were noted in the control or exposed rats, mice or guinea pigs during the exposure period. Upon removal from the chamber, dry rales (1/10) and excessive salivation (2/10) were observed in exposed rats. During the 14-day observation period, excessive salivation was observed in mice (4/10) and nasal discharge (2/10) occurred. Necropsy examination revealed an increased incidence of lung discoloration in treated rats (6/10) and guinea pigs (8/10).
Conclusions	Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute inhalation toxicity in rats.
Data Quality	2 - Valid with restrictions - Vapor concentration not analyzed.
Reference	Esso Research and Engineering (1980). Unpublished Report.
Date last changed	September, 2000

Acute Toxicity

Test Substance CAS No.	Alcohols, C7-9 branched 68526-83-0
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels	OECD 401 Acute oral toxicity Yes 1988 Rats/Wistar Males and Females 5/sex/dose Oral gavage None Single Dose 2000 mg/kg
Remarks on Test Conditions	After being fasted for 12 to 18 hours, animals were administered a single oral gavage dose of 2,000 mg/kg of the undiluted test article. Observations were made four times on day 1; and daily for 14 days.
Results	LD_{50} > 2000 mg/kg
Remarks	Following dosing, the following symptoms were observed: sedation, ventral body position in males, hunched posture, and ruffled fur. However, all animals had recovered within 6 days of dosing. At necropsy, no macroscopic abnormalities were observed.
Conclusions	Under the conditions of this study, Alcohols, C7-9 branched has a low order of toxicity.
Data Quality	1 – Reliable without restrictions
Reference	"Acute oral toxicity study with Alcohols, C7-9 branched in rats," unpublished report (RCC Research and Consulting Co. AG).
Date last changed	September, 2000

Acute Toxicity

Test Substance	Alcohols, C7-9 branched
CAS No.	68526-83-0
Method/Guideline	Other
Type of Study	Acute dermal toxicity
GLP	Pre-GLP
Year	1960
Species/strain	Albino Rabbits
Sex	Males and Females
No. of animals/sex/dose	4 rabbits/sex/dose
Route of administration	Dermal; with occlusive binding
Frequency of treatment	Single 24 hour exposure
Dose/Concentration Levels	83, 262, 820, 2623 mg/kg (undiluted)
Control group and treatment	None
Remarks on Test Conditions	The test substance was applied dermally to rabbits (4/sex/dose) under occlusive binding and removed after 24 hours. The results were converted to weight units by means of the specific gravity. Animals were observed 1, 4, and 24 hours after initial application of Alcohols, C7-9 branched and once daily for the next 7 days. At the termination of the study, survivors were weighed and gross necropsies were performed.
Results	Dermal LD_{50} > 2623 mg/kg
Remarks	Animals in the 83, 262, and 820 mg/kg dose groups exhibited normal appearance and behavior throughout the study. At the highest dose (2623 mg/kg), animals exhibited labored respiration and were inactive. One animal in the high dose group died within 24 hours. The remaining animals in this dose group returned to normal appearance and behavior 2 days after the treatment.
Conclusions	Alcohols, C7-9 branched showed a low order of acute dermal toxicity under the conditions of this study.
Data Quality	1 - Reliable without restrictions
Reference	Hazleton Labs (1960). Acute oral, acute dermal, and acute inhalation toxicity. Unpublished report.
Date last changed	September, 2000

Acute Toxicity

Test Substance	Alcohols, C7-9 branched
CAS No.	68526-83-0
Method/Guideline	Other
Type of Study	Acute inhalation toxicity
GLP	Pre-GLP
Year	1960
Species/strain	Rats/Wistar, Mice/Swiss, Guinea pigs/English Short Hair
Sex	Males
No. of animals/sex/dose	10/species
Route of administration	Inhalation
Vehicle	NA
Frequency of Treatment:	Single 6 hour exposure
Dose/Concentration Levels	Saturated Vapors
Remarks on Test Conditions	Rats, mice, and guinea pigs were exposed to near-saturation levels (200 ppm) of vapors of Alcohols, C7-9 branched in a 500 L stainless steel inhalation chamber for 6 hours. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml of the test substance. Air flow through each bubbler was 18 l/m, and the total flow through the chamber was 36 l/m. Actual chamber concentration was not measured; theoretical chamber concentration was calculated to be 200 ppm. Animals were observed at one-hour intervals during the exposure. Animals were observed 24 hours following exposure and then necropsies were performed.
Results	LC_{50} > 200 ppm
Remarks	There were no deaths during the treatment period. There were no apparent signs of toxicity or alterations to behavior other than blinking in rats and mice. No macroscopic abnormalities were observed at necropsy.
Conclusions	Under the conditions of this study, Alcohols, C7-9 branched has a low order of acute inhalation toxicity in rats, mice and guinea pigs.
Data Quality	2 - valid with restrictions - No analysis of exposure atmosphere.
Reference	Hazleton Labs (1960). Acute oral, acute dermal, and acute inhalation toxicity. Unpublished report.
Date last changed	September, 2000

Genetic Toxicity

Test Substance	2-Ethyl-1-hexanol
CAS No.	104-76-7
Method	Other
Type of Study	Ames Assay
Test System	*S. typhimurium, E. coli*
GLP	Not specified
Year	1985
Species/Strain	*Salmonella typhimurium* /TA98; TA100; TA1535; TA1537; TA1538; *E. coli* WP2uvrA
Metabolic Activation	S9 mixture
Concentrations	1, 5, 10, 50, 100, 500, and 1000 ug/plate.
Statistical methods	Samples were run in duplicate. No further details provided.
Remarks on Test Conditions	2-Ethyl-1-hexanol (98% pure) was dissolved in DMSO at appropriate concentrations. 0.1ml of this mixture was added to 0.1 ml of bacteria and 0.5 ml of either S9 mix (Polychlorinated biphenyl-induced rat liver S9 mixture) or phosphate-buffered saline. Following a 20-minute pre-incubation, the mixtures were combined with agar and incubated for 48 hours. Colonies were scored with an automatic counter. All tests were performed in duplicate. 2-(2-Furyl)-3-(5-nitro-2-furyl)-acrylamide (AF-2), N-ethyl-N'-nitro-N-nitrosoguanidine (ENNG), 9-aminoacridine (9AC), 4-nitroquinoline-1-oxide (4NQO), benzo(a)pyrene (B(a)P), 2-aminoanthracene (2AA), and 2-nitrofluorene (2NF) were used as positive controls. In addition, water and DMSO were used as vehicle controls.
Results	Negative
Remarks for Results	In all of the strains tested, there was no evidence of mutagenicity of 2-ethyl-1-hexanol in the presence or absence of metabolic activation. The number of revertant colonies per plate did not vary significantly between the water, DMSO, or 2-ethyl-1-hexanol samples.
Conclusions	2-Ethyl-1-hexanol is not mutagenic in bacteria under the conditions of this study.
Data Quality	2- Reliable with restrictions (Similar to OECD 471)
Reference	H. Shimizu, Y. Suzuki, N. Takemura, S. Goto, H. Matsushita, (1985) "The Results of Microbial Mutation Test for Forty-Three Industrial Chemicals," *Japanese Journal of Industrial Health*, 27: 400-419.
Date last changed	October 3, 2000

Repeat Dose Toxicity

Test Substance	Iso-octanol
CAS No.	--
Method/Guideline	NA
Type of Study	14-day repeat dose
GLP	Not specified
Year	1984
Species/strain	Rats/Wistar
Sex	Male
No. of animals/sex/dose	5/treatment, 10/control; 1mmol/kg/day of iso-octanol (130 mg/kg/day)
Route of administration	Oral gavage.
Duration of test	14 days
Frequency of treatment	Once daily for 14 days
Vehicle	Polyethylene glycol 300
Statistics	Mean values compared to controls by Student's t-test.
Remarks on Test Conditions	After acclimation for 1 week, five animals received 1mmol/kg/day (130 mg/kg/day) of the test substance by oral gavage and ten animals received only the vehicle, PEG 300, daily for 14 days. Animals were sacrificed after 14 days by halothane overdose and blood was withdrawn by cardiac puncture and analyzed for plasma cholesterol and triglycerides. The liver was removed for histopathological analysis, analysis of catalase, and CN-insensitive palmitoyl CoA oxidation. Testicular weight was also determined.
Results	NOAEL = 130 mg/kg/day
Remarks	Iso-octanol did not significantly change body weight gain, liver to body weight ratio, or testis to body weight ratio when compared to vehicle controls. Iso-octanol did not induce any changes in glycogen vacuolation or fat vacuolation. The activity of peroxisome-associated enzymes and levels of cholesterol and triglyceride were not significantly different between animals treated with iso-octanol and vehicle controls. No hyperlipidemia was observed.
Conclusions	Under the conditions of this study, iso-octanol had a low order of sub-acute toxicity in male rats for the endpoints studied.
Data Quality	2 - Reliable with restrictions - Not a guideline study.
Reference	C. Rhodes, T. Soames, M.D. Stonard, M.G. Simpson, A.J. Vernall, C.R. Elcombe, "The absence of testicular atrophy and in vivo and in vitro effects on hepatocyte morphology and peroxisomal enzyme activities in male rats following the administration of several alkanols," (1984). Toxicology Letters 21: 103-109.
Date last changed	13-Sep-00

Repeat Dose Toxicity

Test Substance	Alcohols, C7-9 branched
CAS No.	68526-83-0
Method/Guideline	Other
Test Type	Repeated Dermal Application
GLP	Pre-GLP
Year	1961
Species/strain	Albino Rabbits
Route of administration	Dermal
Duration of test	12 days
Number of animals	8 rabbits (2/sex/dose)
Dose/Conc. Levels	0.4 g/kg and 2.0 g/kg
Sex	Males and Females
Frequency of treatment	Single Daily treatment for 10 days
Control group	Isopropyl alcohol, 2/sex
Statistical methods	Not specified
Remarks on Test Conditions	Undiluted control and test materials were applied to intact skin of the animals (2/sex/dose). Materials were applied once daily for a total of ten applications with a one-day rest period between the third and fourth and eighth and ninth applications. The exposed skin area of each animal was approximately 10% of the total body surface at the 0.4 g/kg dosage level and approximately 40% of the total body surface at the 2.0 g/kg dosage level. After the first application, exposed skin was covered by rubber dental damming. In subsequent applications, loose gauze and adhesive tape were used to cover the exposed area since the authors felt that the damming itself may have induced some irritation. Each exposure period lasted approximately 18-24 hours. Animals were observed daily throughout the study and body weights were recorded prior to each exposure and at study termination. Clinical hematology and urinalysis were performed at the beginning of the study and 24 hours after the final application of test material. Animals were sacrificed 48 hours after the tenth application, samples of brain, thyroid, lung, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved.
Results	NOAEL for systemic toxicity = 2.0 g/kg
Remarks	Animals in all exposure groups displayed normal appearance and behavior throughout the study. Although a slight decrease in body weight was observed initially, animals regained weight by the end of the study. Repeat application of the control substance, isopropyl alcohol produced slight irritation characterized by slight to moderate erythema, atonia, and desquamation. Repeated application of Alcohols, C7-9 branched resulted in moderate to severe irritation. Fissuring and coriaceous skin were also observed at both the low and high dose levels. Necrosis was observed in the high dose animals as well. Clinical studies did not indicate any other signs of toxicity. There was a general increase in the hematocrit and erythrocyte values at the end of the study.

Conclusions	Under the conditions of this study, Alcohols, C7-9 branched can produce moderate skin irritation following repeated dermal exposures. However, the test material did not produce any evidence of systemic toxicity under the conditions of this study.
Data Quality	2 - Valid with restrictions
Reference	Esso Research and Engineering Company (1961). Repeat Dermal Application of Alcohols, C7-9 branched, Unpublished Report.
Date last changed	September, 2000

Developmental Toxicity

Test Substance	1-Octanol
CAS No.	NR
Method/Guideline	Other
Type of Study	Developmental Toxicity
GLP	Not specified
Year	1989
Species/strain	Rats/Sprague-Dawley
Sex	Pregnant females
No. of animals/sex/dose	15/dose
Route of administration	Inhalation
Frequency of treatment	7 hrs/day; Gestation days 1-19
Dose/Concentration Levels	400 mg/m^3
Control group and treatment	15 sham-exposed rats
Statistical methods	MANOVA, ANOVA, Kruskal-Wallis test
Remarks on Test Conditions	Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the test substance was ≥ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heat compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 3500 mg/m^3. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by CO_2 asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects.
Results	Maternal and Developmental NOAEL ≥ 400 mg/m^3

Remarks	No treatment-related effects were observed in dams. There were no significant differences in maternal weight gain, feed consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. The number of corpora lutea and resorptions, the sex ratio, and fetal weights were not significantly different between the control and treated groups.
Conclusions	Under the conditions of this study, exposure of pregnant rats to saturated vapors of 1-Octanol does not induce maternal or fetal toxicity.
Data Quality	2 - Reliable without restrictions
Reference	B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology assessment of 1-Octanol, 1-Nonanol, and 1-Decanol administered by inhalation to rats." (1990) Journal of the American College of Toxicology 9(1): 93-97. NIOSH, Division of Biomedical and Behavioral Sciences.
Date last changed	February, 2001

Developmental Toxicity

Test Substance	Alcohols, C7-9 branched
CAS No.	68526-83-0
Method/Guideline	OECD 414
Type of Study	Developmental Toxicity
GLP	Yes
Year	1994
Species/strain	Rat/Sprague-Dawley
Sex	Females
No. of animals/dose	25/dose
Route of administration	Oral gavage
Exposure period	GD 6-15
Dose/Concentration Levels	100, 500, and 1000 mg/kg/day
Control group and treatment	Carrier only - corn oil
Statistical methods	Nested analysis of covariance, Least Significant Difference (LSD), Chi-square, Fisher Exact test, Armitage's test.
Remarks on Test Conditions	Mated females were assigned to dose groups of 100, 500, and 1000 mg/kg/day or to a corn oil-only group (25/dose). The test substance was administered in volumes of 5 ml/kg. Body weight and food consumption measurements were made on GD 0, 6, 9, 12, 15, 18, and 21. The animals were examined for viability twice daily during the treatment period and once daily thereafter. Clinical observations were made daily during gestation. On GD 21, animals were sacrificed and cesarean sections and necropsies were performed. Uterine weights with ovaries attached were recorded, uterine contents were examined, and implantation data were recorded. All live fetuses were weighed, sexed externally, and examined externally for gross malformations. Approximately one-half of the fetuses were prepared for examination of abnormalities in the head and the other half were preserved for examination of skeletal abnormalities.
Results	Maternal NOAEL = 500 mg/kg/day Fetal NOAEL = 1000 mg/kg/day
Remarks	One animal in the high dose group was euthanized in moribund condition on GD 9. The animal had extreme abdominal staining just prior to death, but there were no significant findings at postmortem examination and the cause of morbidity was therefore not established. Adverse clinical signs were observed in 8 of the 24 dams in the high dose group. These signs included emaciation, decreased food consumption, abdominal/anogenital staining, rales, hypoactivity, and little or no stool. The symptoms were transient and generally were not observed following cessation of dosing. The remaining dams in the high dose group had incidental findings such as alopecia, but otherwise appeared normal throughout the study. There were no observable abnormalities in dams of the middle and low dose groups throughout the gestational period. In the high dose group, statistically significant decreased body weight gain and food consumption were observed from GD 6-9 and GD6-15 compared to controls. However, these effects subsided after cessation of treatment and body weight and food consumption for the overall gestational period (GD 6-21) were not significantly different between the high dose group and controls. There were no maternal findings at necropsy that were judged to be the result of treatment with Alcohols, C7-9 branched. For the most part, uterine implantation parameters were equivalent between the treated and control groups.

Remarks, cont'd	There were slight differences between the high dose group and the control group in the number of post-implantation losses and resorptions, however these differences were not statistically significant and were deemed to be due to the poor health of the dams. Mean fetal body weight was equivalent between treated and control fetuses of both sexes. Three low dose, two mid dose, and one high dose fetus were stunted. There were no statistically significant differences in mean skeletal ossification sites and in total or individual external, visceral, or skeletal malformations between control and treated groups. There were statistically significant increases in total fetuses with skeletal variations and in the incidence of hypoplastic skull bones in the high dose group when compared to controls. These findings were slightly higher than the historical control range of the lab and were not observed with litter-based analysis. Statistically significant increases in the number of lumbar ribs were observed in the middle and high dose groups. However, due to the lack of embryotoxicity observed in this study, these findings were attributed to maternal toxicity observed during treatment.
Conclusions	Under the conditions of this study, Alcohols, C7-9 branched induces maternal toxicity at concentrations that are not embryotoxic.
Data Quality	1 - Reliable without restrictions
Reference	Exxon Biomedical Sciences, Inc. (1994). Developmental Toxicity Study in Rats, Unpublished report.
Date last changed	February, 2001

Acute Toxicity

Test Substance	Alcohols, C8-10 iso, C9 rich
CAS No.	68526-84-1
Method/Guideline	NA
Type of Study	Acute oral toxicity
GLP	Pre-GLP
Year	1968
Species/strain	Rats/Sprague-Dawley
Sex	Males
No. of animals/sex/dose	5/dose
Route of administration	Gastric Intubation
Vehicle	None
Frequency of Treatment	Single Exposure
Dose/Concentration Levels	34.6, 120, 417, 1450, 5000 or 10,000 mg/kg
Control group and Treatment	None
Remarks on Test Conditions	After a three to four hour fasting period, groups of 5 rats (approximately 252-295 grams) received the undiluted test material at doses of 34.6, 120, 417, 1450, 5000 or 10,000 mg/kg body weight. Observations were recorded immediately after dosing; at one, four and 24 hours; and once daily for a total of 14 days.
Results	LD_{50} = 2979 mg/kg
Remarks	No deaths occurred in the 34.6, 120, 417, and 1450 mg/kg groups throughout the study. Two of the five animals in the 5000 mg/kg group died within 24 hours and all of the animals in the 10,000 mg/kg group died within 24 hours. Depression, labored respiration and evidence of excessive urination and/or diarrhea were observed at the 5,000 and 10,000 mg/kg dose levels. These signs of toxicity were observed within one hour of administration. At necropsy, abscessed lungs, dark red lungs and a dark zone between the renal cortex and medulla were observed in animals from the 5,000 and 10,000 mg/kg dose levels.
Conclusions	Under conditions of this study, Alcohols, C8-10 iso, C9 rich have a low order of acute oral toxicity in rats.
Data Quality	2 - Valid with restrictions (Pre-GLP)
Reference	Esso Research and Engineering (1968). Unpublished report.
Date last changed	September, 2000

Acute Toxicity

Test Substance	Alcohols, C8-10 iso, C9 rich
CAS No.	68526-84-1
Method/Guideline	Other
Type of Study	Acute dermal toxicity
GLP	Pre-GLP
Year	1968
Species/strain	Rabbits/New Zealand White
Sex	Males and Females
No. of animals/sex/dose	2/sex/dose
Route of administration	Dermal
Frequency of Treatment	Single Exposure
Dose/Concentration Levels	50, 200, 794 and 3,160 mg/kg
Remarks on Test Conditions	A single application of the test material was made to four groups of four rabbits (2.0 to 2.8 kg) at doses of 50, 200, 794 and 3160 mg/kg. The material was applied to abraded abdominal skin under occlusive dressing. Observations were recorded immediately following application; at one, four and 24 hours; and once daily thereafter for a total of 14 days.
Results	LD_{50} > 3,160 mg/kg of body weight.
Remarks	No deaths were observed at any timepoint in this study. No evidence of systemic toxicity was observed. Dose-related moderate to severe skin irritation was produced. For all of the doses tested, no compound-related alterations were observed at necropsy.
Conclusions	Under the conditions of this study, Alcohols, C8-10 iso, C9 rich has a low order of acute dermal toxicity in rats.
Data Quality	2 - Valid with restrictions (Pre-GLP)
Reference	Esso Research and Engineering (1968). Unpublished report.
Date last changed	September, 200

Repeat Dose Toxicity

Test Substance	Isononanol
CAS No.	NR
Method/Guideline	Other
Type of Study	14-day repeated dose
GLP	Not specified
Year	1983
Species/strain	Wistar Rats
Sex	Male
No. of animals/sex/dose	5/treatment, 10/control; 1mmol/kg/day of isononanol (144 mg/kg/day)
Route of administration	Oral gavage.
Frequency of treatment	Once daily for 14 days
Vehicle	Polyethylene glycol 300
Statistical methods	Mean values compared to controls by Student's t-test.
Remarks on Test Conditions	After acclimation for 1 week, five animals received 1mmol/kg/day (130 mg/kg/day) of the test substance by oral gavage and ten animals received only the vehicle, PEG 300, daily for 14 days. Animals were sacrificed after 14 days by halothane overdose and blood was withdrawn by cardiac puncture and analyzed for plasma cholesterol and triglycerides. The liver was removed for histopathological analysis, analysis of catalase, and CN-insensitive palmitoyl CoA oxidation. Testicular weight was also determined.
Results	NOAEL ≥ 144 mg/kg/day
Remarks	Isononanol did not significantly change body weight gain, liver to body weight ratio, or testis to body weight ratio when compared to vehicle controls. Isononanol did not induce any changes in glycogen vacuolation or fat vacuolation. The levels of cholesterol and triglyceride were not significantly different between animals treated with isononanol and vehicle controls. There was a slight induction of palmitoyl CoA oxidase activity. However, the activity of other peroxisome-associated enzymes was not affected and overall peroxisome number was not effected. No hyperlipidemia was observed.
Conclusions	Under the conditions of this study, isononanol has a low order of sub-acute toxicity in male rats for the endpoints studied.
Data Quality	2 - Valid with restrictions
Reference	C. Rhodes, T. Soames, M.D. Stonard, M.G. Simpson, A.J. Vernall, C.R. Elcombe, "The absence of testicular atrophy and in vivo and in vitro effects on hepatocyte morphology and peroxisomal enzyme activities in male rats following the administration of several alkanols," (1984). Toxicology Letters **21**: 103-109.
Date last changed	13-Sep-00

Developmental Toxicity

Test Substance	Isononylalcohol 1
CAS No.	68515-81-1
Method/Guideline	OECD 414
Type of Study	Developmental Toxicity
GLP	Yes
Year	1989
Species/strain	Rats/Wistar
Sex	Females
No. of animals/sex/dose	10/dose
Route of administration	Oral gavage
Vehicle	Aqueous emulsion in 0.005% Cremophor EL
Frequency of Treatment	Gestation days 6-15
Dose/Concentration Levels	144, 720, 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day)
Control group and Treatment	Control Group 1: Doubly distilled water Control Group 2: Doubly distilled water with 0.005% Cremophor EL
Statistical Methods	Dunnett's test, Fisher's exact test
Remarks on Test Conditions	The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isononylalcohol 1 or Isononylalcohol 2 were administered to rats (10/dose) on days 6 through 15 of gestation at doses of 144, 720, or 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings.
Results	NOAEL = 144 mg/kg/day (Maternal and Fetal)
Remarks	At the lowest dose level, no maternal toxicity was observed. There were an increased number of fetuses with hydroureter. However, the significance of this endpoint as an indicator of marginal developmental toxicity is questionable. At both the 144 and 720 mg/kg/day dose levels, there were no effects on the following parameters: uterine weight, conception rate, mean number of corpora lutea and implantation sites, pre- and post-implantation loss, number of resorptions, and viable fetuses. At the 720 mg/kg/day level, the following signs of maternal toxicity were observed - reduced food consumption, reduced body weight, unsteady gait, and reddish nasal discharge. Fetal effects included a slightly reduced mean fetal body weight and an increased number of fetuses with hydroureter. Signs of maternal toxicity at the 1440 mg/kg/day level included reduced rood consumption and mean body weight, severe clinical symptoms like abdominal or lateral position, and unsteady gait. In addition, 7 of the animals found dead by gestation day 11 and the remaining 3 were sacrificed in moribund condition by gestation day 10. At necropsy, all animals had light brown-gray discoloration of the liver and some had evidence of lung edema and petechiae in the lungs. Because of the death of all dams within the high dose group, no data were available to assess uterus weight, reproduction parameters, or fetal effects.

Conclusions	When administered by oral gavage under the conditions of this study, Isononylalcohol 1 causes embryo/fetal toxicity at doses that induce overt maternal toxicity. In addition, Isononylalcohol 1 does not alter reproductive parameters at doses that are not maternally toxic.
Data Quality	2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed.
Reference	Report: Study of the Prenatal Toxicity of Isononylalcohol 1 and Isononylalcohol 2 in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000247.
Date last changed	February, 2001

Developmental Toxicity

Test Substance	Isononylalcohol 2
CAS No.	68515-81-1
Method/Guideline	OECD 414
Type of Study	Developmental Toxicity
GLP	Yes
Year	1989
Species/strain	Rats/Wistar
Sex	Females
No. of animals	10/group
Route of administration	Oral gavage
Frequency of Treatment	Gestation days 6-15
Dose/Concentration Levels	144, 720, 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day)
Control Group and Treatment	Control Group 1: Doubly distilled water Control Group 2: Doubly distilled water with 0.005% Cremophor EL
Statistical methods	Dunnett's test, Fisher's exact test
Remarks on Test Conditions	The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isononylalcohol 1 or Isononylalcohol 2 were administered to rats (10/dose) on days 6 through 15 of gestation at doses of 144, 720, or 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings.
Results	NOAEL = 144 mg/kg/day
Remarks	At the lowest dose level, no maternal or fetal toxicity was observed. In addition, there were no changes in reproductive parameters. At the 720 mg/kg/day level, signs of maternal toxicity included unsteady gait, piloerection, salivation, and reduced body weight gain and food consumption. There was also an increased frequency of fetuses with hydroureter at this level. At this level, there were no significant changes in reproductive parameters. Although there was an increased number of late resorptions, this number was within the range of biologic variation, was not dose-dependent, and was therefore considered incidental. At the highest dose level, dams exhibited marked decreases in weight gain and food consumption, and displayed severe clinical symptoms, including unsteady gait, apathy, and abdominal or lateral position. One animal was found dead on gestation day 9 and two other dams were sacrificed in moribund condition on gestation days 8 and 109. At necropsy, light brown-gray discoloration of the liver, lung edema, and petechiae in the lungs, heart, or bladder were observed. Fetuses from the high dose group had markedly reduced mean fetal body weight, increased frequency of hydroureter, and a higher frequency of fetuses with skeletal variations and retardations. At the highest dose, there were no changes in fertility parameters.

Conclusions	When administered by oral gavage under the conditions of this study, Isononylalcohol 2 causes embryo/fetal toxicity at doses that induce overt maternal toxicity. In addition, Isononyl alcohol 2 does not alter fertility parameters at doses that are not maternally toxic.
Data Quality	2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed.
Reference	Report: Study of the Prenatal Toxicity of Isononylalcohol 1 and Isononylalcohol 2 in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000247.
Date last changed	February, 2001

Developmental Toxicity

Test Substance	1-Nonanol
CAS No.	--
Method/Guideline	Other
Type of Study	Developmental Toxicity
GLP	Not specified
Year	1989
Species/strain	Rats/Sprague-Dawley
Sex	Pregnant females
No. of animals/sex/dose	15 dams/dose
Route of administration	Inhalation
Frequency of treatment	7 hrs/day; Gestation days 1-19
Dose/Concentration Levels	150 mg/m^3 (Saturated vapors)
Control group and treatment	15 sham-exposed rats
Statistical methods	MANOVA, ANOVA, Kruskal-Wallis test
Remarks on Test Conditions	Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the test substance was ≥ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heat compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 3500 mg/m^3. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by CO_2 asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects.
Results	NOAEL = 150 mg/m^3
Remarks	No treatment-related effects were observed in dams. There were no statistically significant differences in maternal weight gain, feed consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. There were no statistically significant differences between the mean number of corpora lutea and resorptions, the sex ratio, and the mean fetal weights between the control and treated groups.

Conclusions	Under the conditions of this study, exposure of pregnant rats to saturated vapors of 1-Nonanol does not induce maternal or fetal toxicity.
Data Quality	2 - Reliable with restrictions - Similar to guideline study; only one exposure level.
Reference	B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology assessment of 1-Octanol, 1-Nonanol, and 1-Decanol administered by inhalation to rats." (1990) Journal of the American College of Toxicology **9(1)**: 93-97. NIOSH, Division of biomedical and behavioral sciences
Date last changed	February, 2001

Acute Toxicity

Test Substance	Alcohols, C9-C11 iso, C10 rich
CAS No.	68526-85-2
Method/Guideline	Other
Type of Study	Acute oral toxicity
GLP	Pre-GLP
Year	1960
Species/strain	Rats/Sprague-Dawley
Sex	Male
No. of animals/sex/dose	5/dose
Route of administration	Oral gavage
Vehicle	Corn oil
Frequency of Treatment	Single Treatment
Dose/Concentration Levels	0.1, 1.0, 10.0, 30.0% volume/volume emulsion in corn oil (Equivalent to 26, 82, 260, 820, 2600, 8200 mg/kg)
Control group and Treatment	For comparison, untreated animals were necropsied at the end of the study.
Remarks on Test Conditions	Prior to dosage, food was withheld from the animals for three to four hours. The animals were observed for gross effects and mortality at one, four, and twenty-four hours, and once daily thereafter up until seven days. Gross necropsies were performed at the end of the observation period and samples of liver, kidney, brain, and blood were taken from untreated control animals and from all surviving animals at the 820 and 2600 mg/kg dose levels.
Results	LD_{50} = 4626 mg/kg
Remarks	5/5 animals died within the first four hours following exposure to 8200 mg/kg. Animals in all other dose groups survived until the end of the study. At the one and four-hour intervals, animals in the 260 and 820 mg/kg dose groups were inactive and displayed labored respiration, ataxia, and sprawling of the limbs. At the 24-hour interval, animals had oily fur. After approximately 48-hours after dosing, most animals in these groups returned to normal appearance and behavior. At the 2600 mg/kg dose level, animals exhibited similar symptoms as above but also showed lacrimation and depressed righting and placement reflexes. Animals in this dose group also returned to normal appearance and behavior after 24 hours. At the highest dose, animals initially exhibited labored respiration, ataxia, and sprawling of the limbs, which was followed by a comatose state and death within 4 hours of exposure. The surviving animals at the five lower dose levels (26, 82, 260, 820, 2600 mg/kg) had weight gain that was within the normal range. Gross autopsies performed on animals that died (5/5 in 8200 mg/kg group) revealed congested lungs, kidneys, and adrenals, and dark-appearing spleens. No abnormalities were observed in the surviving animals at necropsy. Therefore, a histopathologic analysis was not performed.
Conclusions	Under the conditions of this study, Alcohols, C9-C11 iso, C10 rich has a low order of toxicity.
Data Quality	2 - Valid with restrictions (Pre-GLP).
Reference	Esso Research and Engineering (1960). Unpublished report.
Date last changed	October, 2000

Acute Toxicity

Test Substance	Alcohols, C9-C11 iso, C10 rich
CAS No.	68526-85-2
Method/Guideline	Other
Type of Study	Acute dermal toxicity
GLP	Pre-GLP
Year	1960
Species/strain	Rabbits/Albino
Sex	Males and Females
No. of animals	2/sex/dose
Route of administration	Dermal
Frequency of Treatment	Single Dose
Dose/Concentration Levels	80, 260, 820, and 2600 mg/kg
Remarks on Test Conditions	A single application of the test material was given to four groups (2/sex/dose) of four rabbits at doses of 80, 260, 820, and 2600 mg/kg. The material was applied under occlusive dressing to intact abdominal skin. Observations were recorded at one, four and 24 hours; and once daily thereafter for a total of 7 days. Samples of liver, kidney, brain and blood were taken from four untreated control albino rabbits and from each surviving animal at the 820 and 2600 mg/kg dose level.
Results	The acute dermal LD50 is > 2600 mg/kg
Remarks	No deaths were observed during this study. Mild to moderate erythema and edema were observed in animals at the three lower dose levels. Marked erythema and edema were observed at the highest dose level. Edema in each animal subsided within 3 days. Erythema in animals at the high dose group diminished in intensity but did not subside completely during the observation period. Autopsies performed following sacrifice revealed no gross pathological findings in any animal. Therefore, a histopathologic analysis was not performed.
Conclusions	Under conditions of this study, Alcohols, C9-C11 iso, C10 rich has a low order of acute dermal toxicity in rats.
Data Quality	2 - Valid with restrictions (Pre-GLP).
Reference	Esso Research and Engineering (1960). Unpublished report.
Date last changed	September, 2000

Developmental Toxicity

Test Substance	Isodecanol
CAS No.	25339-17-7
Method/Guideline	OECD 414
Type of Study	Developmental Toxicity
GLP	Yes
Year	1989
Species/strain	Wistar rats
Sex	Females
No. of animals/sex/dose	10/dose
Route of administration	Oral gavage
Frequency of treatment	Gestation day 6-15
Dose/Concentration Levels	158, 790, 1580 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day)
Statistical methods	Dunnett's test, Fisher's exact test
Remarks on Test Conditions	The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isodecanol was administered at doses of 158, 790, or 1580 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings.
Results	Maternal NOAEL = 158 mg/kg, Fetal NOAEL = 790 mg/kg
Remarks	At the lowest dose level, no adverse effects were observed in the dams or the fetuses as a result of exposure to the test compound. There were also no differences from controls with respect to the following reproductive parameters: conception rate, mean number of corpora lutea and implantation sites, pre- and post-implantation loss, number of resorptions, number of viable fetuses, placental weight, and sex distribution of the fetuses. Dams of the middle dose group exhibited reduced body weight gain and did not consume as much food as the control animals. Animals in the middle dose group also had an unsteady gait and reddish nasal discharge. No embryo or fetotoxic effects were observed at this dose. In addition, there were no changes in fertility parameters at the middle dose. Treatment with the highest dose of isodecanol resulted in statistically significant decreases in food consumption, body weight, and body weight gain in the dams. Three animals in the high dose group were found dead on gestation days 9 and 10. A fourth dam was sacrificed in moribund condition on gestation day 10. All of the dams in the high dose group had clinical symptoms that included nasal discharge, salivation, and signs of CNS depression.

Results, continued	At necropsy, the liver was light brown-gray and the mean gravid uterus weight was reduced. The lungs displayed signs of edema and emphysema. There were statistically significant increases in the number of resorptions in the high dose group as well as significantly reduced mean fetal body weight. However, there were no other statistically significant changes in reproductive parameters. Two litters had 2 anedeous fetuses. In addition, there were an increased number of fetuses with skeletal retardations.
Conclusions	Isodecanol is embryo and fetotoxic at doses that produce overt toxicity in the dam. In the absence of maternal toxicity, isodecanol is not embryo or fetotoxic under the conditions of this study. Furthermore, isodecanol does not alter fertility parameters at doses that are not maternally toxic.
Data Quality	2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed.
Reference	Report: Study of the Prenatal Toxicity of Isodecanol, 2-Ethylhexanol, and 711 Alcohol (T.C.) in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000245.
Date last changed	October, 2000

Developmental Toxicity

Test Substance	1-Decanol
CAS No.	--
Method/Guideline	Other
Type of Study	Developmental Toxicity
GLP	Not specified
Year	1989
Species/strain	Sprague-Dawley Rats
Sex	Pregnant females
No. of animals/sex/dose	15 dams/treatment
Route of administration	Inhalation
Frequency of treatment	7 hrs/day; Gestation days 1-19
Dose/Concentration Levels	100 mg/m^3 (Saturated vapors)
Control group and treatment	15 sham-exposed rats
Statistical methods	MANOVA, ANOVA, Kruskal-Wallis test
Remarks on Test Conditions	Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Animals had free access to food and water. Exposures were conducted in Hinners-type chambers. The purity of the test substance was ≥ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heat compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 3500 mg/m^3. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by CO_2 asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects.
Results	NOAEL = 100 mg/m^3
Remarks	No treatment-related effects were observed in dams. There were no significant differences in maternal weight gain, feed consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. The number of corpora lutea and resorptions, the sex ratio, and fetal weights were not significantly different between the control and treated groups.

Conclusions	Under the conditions of this study, exposure of pregnant rats to vapors of 1-Decanol does not induce maternal or fetal toxicity.
Data Quality	2 - Reliable with restrictions - Similar to guideline study; only one exposure level.
Reference	B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology assessment of 1-Octanol, 1-Nonanol, and 1-Decanol administered by inhalation to rats." (1990) Journal of the American College of Toxicology **9(1)**: 93-97. NIOSH, Division of Biomedical and Behavioral Sciences
Date last changed	February, 2001

Developmental Toxicity

Test Substance	C7-9-11 Alcohol The test material consists mainly of linear alcohols and also contains significant amounts of alpha-methyl branched alcohols ranging in carbon chain length from C7 to C11.
CAS No.	85566-14-9
Method/Guideline	OECD 414
Type of Study	Developmental Toxicity
GLP	Yes
Year	1989
Species/strain	Rats/Wistar
Sex	Females
No. of animals/sex/dose	10/dose
Route of administration	Oral gavage
Frequency of treatment	Gestation day 6-15
Dose/Concentration Levels	144, 720, 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day)
Statistical methods	Dunnett's test, Fisher's exact test
Remarks on Test Conditions	The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isodecanol was administered at doses of 144, 720, or 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings.
Results	Maternal NOAEL ≥ 1,440 mg/kg/day Fetal NOAEL ≥ 1,440 mg/kg/day
Remarks	No adverse effects were observed at any dose of C7-9-11 Alcohol. This included changes in body weight and food consumption by the dams, reproductive parameters, and signs of fetal toxicity.
Conclusions	C7-9-11 Alcohol does not produce signs of toxicity in the dam or the fetus. C7-9-11 Alcohol is not embryo or fetotoxic under the conditions of this study.
Data Quality	2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed.
Reference	Report: Study of the Prenatal Toxicity of Isodecanol, 2-Ethylhexanol, and 711 Alcohol (T.C.) in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000245.
Date last changed	June, 2001

Acute Toxicity

Test Substance	Alcohols, C11-14 iso, C13 rich
CAS No.	68526-86-3
Method/Guideline	OECD 401
Type of Study	Acute oral toxicity
GLP	Yes
Year	1988
Species/strain	Rats/Wistar
Sex	Males and Females
No. of animals/sex/dose	5/sex/dose
Route of administration	Oral Gavage
Vehicle	None
Frequency of Treatment	Single Dose
Dose/Concentration Levels	2000 mg/kg
Control group and Treatment	None
Remarks on Test Conditions	The testing procedure used in this study is in accordance with OECD Guidelines 401. After being fasted for 12 to 18 hours, male and female rats were administered a single oral gavage dose of 2,000 mg/kg of the test article. Observations were made four times on day 1; and daily for 14 days. Animals were necropsied at the termination of the study.
Results	LD_{50} > 2,000 mg/kg.
Remarks	There were no deaths in males or females. Clinical signs of toxicity that were observed included sedation, diarrhea and dyspnea (males). There were no macroscopic changes observed at necropsy.
Conclusions	Under the conditions of this study, Alcohols, C11-14 iso, C13 rich has a low order of acute oral toxicity in rats.
Data Quality	1 - Valid without restrictions
Reference	Research and Consulting Co., (1988). Acute Oral Toxicity Study with Alcohols, C11-14 iso, C13 rich in Rats, Unpublished report.
Date last changed	September, 2000

Genetic Toxicity

Test Substance	1-Dodecanol
CAS No.	112-53-8
Method	Other
Type of Study	Ames Assay
Test system	*S. typhimurium, E. coli*
GLP	Not specified
Year	1985
Species/Strain	*Salmonella typhimurium* /TA98; TA100; TA1535; TA1537; TA1538; *E. coli* WP2uvrA
Metabolic Activation	Yes
Concentrations	0.01, 0.05, 0.1, 0.5, 1, 5, 10, and 50 ug/plate.
Statistical methods	Samples run in duplicate. No further details provided.
Remarks on Test Conditions	1-dodecanol (90% pure) was dissolved in DMSO at appropriate concentrations. 0.1ml of this mixture was added to 0.1 ml of bacteria and 0.5 ml of either S9 mix (polychlorinated biphenyl-induced rat liver S9 mixture) or phosphate-buffered saline. Following a 20-minute pre-incubation, the mixtures were combined with agar and incubated for 48 hours. Colonies were scored with an automatic counter. All tests were performed in duplicate. 2-(2-Furyl)-3-(5-nitro-2-furyl)acrylamide (AF-2), N-ethyl-N'-nitro-N-nitrosoguanidine (ENNG), 9-aminoacridine (9AC), 4-nitroquinoline-1-oxide (4NQO), benzo(a)pyrene (B(a)P), 2-aminoanthracene (2AA), and 2-nitrofluorene (2NF) were used as positive controls. In addition, water and DMSO were used as vehicle controls.
Results	Negative.
Remarks for Results	There was no evidence of mutagenicity of 1-dodecanol in the presence or absence of metabolic activation in all of the strains tested. The number of revertant colonies per plate did not vary significantly between the water, DMSO, or 1-dodecanol samples.
Conclusions	1-Dodecanol was not mutagenic in bacteria under the conditions of this study.
Data Quality	2- Reliable with restrictions (Similar to OECD 471)
Reference	H. Shimizu, Y. Suzuki, N. Takemura, S. Goto, H. Matsushita, (1985) "The Results of Microbial Mutation Test for Forty-Three Industrial Chemicals," *Japanese Journal of Industrial Health*, **27**: 400-419.
Date last changed	October 3, 2000

Alkyl Alcohols C6-C13 Category

Robust Summaries
Environmental Fate and Effects

Prepared by:

ExxonMobil Chemical Company

November 15, 2001

Table of Contents

CAS # 68526-79-4; Hexanol, branched and linear
Fish Acute Toxicity - Flow Through

CAS # 70914-20-4; Alcohols C6-8, branched
Fish Acute Toxicity - Flow Through
Invertebrate Acute Toxicity

CAS #68526-83-0; Alcohols C7-9, branched
Fish Acute Toxicity - Flow Through
Invertebrate Acute Toxicity
Manometric Respirometry
N-Octanol/Water Partition Coefficient

CAS # 68526-84-1; Alcohols C8-10 iso, C9 rich
Fish Acute Toxicity
Invertebrate Acute Toxicity
Algal Toxicity
N-Octanol/Water Partition Coefficient

CAS #68526-85-2; Alcohols C9-11 iso, C10 rich
Fish Acute Toxicity
Manometric Respirometry
N-Octanol/Water Partition Coefficient
Water Solubility

CAS #68526-86-3; Alcohols C11-14 iso, C12 rich
Fish Acute Toxicity
Invertebrate Acute Toxicity
Manometric Respirometry
N-Octanol/Water Partition Coefficient

CAS #68526-86-3; Alcohols C11-14 iso, C13 rich
Fish Acute Toxicity
Invertebrate Acute Toxicity
Manometric Respirometry
N-Octanol/Water Partition Coefficient
Water Solubility

Fish Acute Toxicity

Test Substance:	Hexanol branched and linear
CAS No.	68526-79-4
Method/Guideline:	No Data
Year (guideline):	No Data
Type (test type):	Flow Through Acute Fish Toxicity Test
GLP:	No Data
Year (study performed):	1980
Species:	Fathead Minnow (*Pimephales promelas*)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method: (FT - ME)	Trimmed Spearman Karber Method
Test Conditions: (FT - TC) • Note: **Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Treatment solutions were prepared by diluting a 3720mg/L stock solution. Nominal hexanol treatment levels were 41, 68, 113, 189, 315mg/L, which measured 26.7, 49.2, 90.6, 170.0, and 261.5mg/L, respectively. Control/dilution water was EPA Duluth laboratory water. Fifty fish were tested per treatment, divided into two replicates. Treatment volume = 6.3L. Test parameters were as follows: temperature=26.2 Deg C; dissolved oxygen = 6.2mg/L; pH = 7.6; fish age = 28 days old; fish mean wt = 0.117g; fish mean length = 19.7mm; fish loading = 0.464g/L/day. Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA.
Results: (FT - RS) Units/Value:	96 hour LC50 = 97.7 mg/L (95% CI 89.7 to 106) based upon measured values
• Note: **Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Analytical method used was Gas-Liquid Chromatography.

Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
26.7	0
49.2	0
90.6	20
170.0	50
261.5	50

* 50 fish added at test initiation

Conclusion: **(FT - CL)**	
Reliability: **(FT - RL)**	(1) Reliable without restriction
Reference: **(FT - RE)**	Brooke, L. T. et al. 1984. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. I. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, WS, USA.
Other (source): **(FT - SO)**	ExxonMobil Biomedical Sciences, Inc.

Fish Acute Toxicity

Test Substance:	Alcohols C6-8, branched
CAS No.	70914-20-4
Method/Guideline:	No Data
Year (guideline):	No Data
Type (test type):	Flow Through Acute Fish Toxicity Test
GLP:	No Data
Year (study performed):	1985
Species:	Fathead Minnow (*Pimephales promelas*)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method: (FT - ME)	Trimmed Spearrman Karber Method
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Treatment solutions were prepared by diluting a 1400mg/L stock solution. Nominal heptanol treatment levels were 12.5, 19.3, 29.7, 45.7, 70.3mg/L, which measured 12.5, 18.1, 28.5, 43.6, and 70.8mg/L, respectively. Control/dilution water was EPA Duluth laboratory water. Twenty fish were tested per treatment. Treatment volume = 2.0L. Test parameters were as follows: temperature=25.6 Deg C; dissolved oxygen = 7.1mg/L; pH = 7.7; fish age = 31 days old; fish mean wt = 0.100g; fish mean length = 18.1mm; fish loading = 1.0g/L/day. Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA.
Results: (FT - RS) **Units/Value:**	96 hour LC50 = 34.5 mg/L (95% CI 33.1 to 36.0) based upon measured values
• **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Analytical method used was Gas-Liquid Chromatography.

Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
12.5	0
18.1	1
28.5	0
43.6	20
70.8	20

* 20 fish added at test initiation

Conclusion: (FT - CL)	
Reliability: (FT - RL)	(1) Reliable without restriction
Reference: (FT - RE)	Geiger, D.L. et al. 1986. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. III. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, WS, USA.
Other (source): (FT - SO)	ExxonMobil Biomedical Sciences, Inc.

Invertebrate Acute Toxicity

Test Substance:	Alcohol C6-8, branched
CAS No.	70914-20-4
Method/Guideline:	Concept rules of the Dutch Standardization Institute (Adema, 1978)
Type (test type):	Daphnid Acute Toxicity Test
GLP:	No Data
Year (study performed):	1978
Species:	Water Flea (*Daphnia magna*)
Analytical Monitoring:	No
Exposure Period:	48 hour
Statistical Method:	No Data
Test Conditions: • **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**	Tests using 15 different chemicals, including n-Heptanol, were performed at two different laboratories. Lab I was the National Institute of Public Health, Bilthoven, The Netherlands; Lab II was the Central Laboratory, T.N.O., Delft, The Netherlands. The tests were conducted using standardized tests methods proposed by the Dutch Standardization Institute (Adema, 1978). The tests were conducted in duplicate to determine the reprodicibility of the results. Organisms were supplied by in-house cultures. Age = <24 hours old.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	48-hour EC50 = 63 mg/L, based upon nominal concentrations of the test chemicals.
Conclusion:	Test substance is considered to have moderate acute toxicity
Reliability:	Code 2, Reliable with Restrictions
Reference:	Canton, J.H. and D.M.M. Adema. 1978. Reproducibility of Short-term and Reproduction Toxicity Experiments with *Daphnia magna* and Comparison of the Sensitivity of *Daphnia magna* with *Daphnia pulex* and *Daphnia cucullata* in Short-term Experiments. *Hydrobiologia*, **59**:2, pp. 135-140.

Other (**reference**)	Adema, D.M.M. 1978. Daphnia magna as Test Organism in Acute and Chronic Toxicity Experiments. *Hydrobiologia*, **59**:2, pp. 125-134.
Other (**source**):	ExxonMobil Biomedical Sciences, Inc.

Fish Acute Toxicity

Test Substance:	Alcohols C7-9, branched
CAS No.	68526-83-0
Method/Guideline:	No Data
Year (guideline):	No Data
Type (test type):	Flow Through Acute Fish Toxicity Test
GLP:	No Data
Year (study performed):	1986
Species:	Fathead Minnow (*Pimephales promelas*)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method: (FT - ME)	Trimmed Spearman Karber Method
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Treatment solutions were prepared by diluting a 275mg/L stock solution. Nominal octanol treatment levels were 8.6, 10.8, 13.5, 16.9, 21.1mg/L, which measured 8.8, 10.7, 12.7, 16.5, and 20.4mg/L, respectively. Control/dilution water was EPA Duluth laboratory water. Twenty fish were tested per treatment. Treatment volume = 2.0L. Test parameters were as follows: temperature=25.3 Deg C; dissolved oxygen = 7.1mg/L; pH = 7.7; fish age = 28 days old; fish mean wt = 0.075g; fish mean length = 16.5mm; fish loading = 0.75g/L/day. Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA.
Results: (FT - RS) **Units/Value:**	96 hour LC50 = 14.0 mg/L (95% CI 13.6 to 14.5) based upon measured values
• **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Analytical method used was Gas-Liquid Chromatography.

Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
8.8	0
10.7	1
12.7	2
16.5	20
20.4	20

* 20 fish added at test initiation

Conclusion: (FT - CL)	
Reliability: (FT - RL)	(1) Reliable without restriction
Reference: (FT - RE)	Geiger, D.L. et al. 1988. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. IV. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, WS, USA.
Other (source): (FT - SO)	ExxonMobil Biomedical Sciences, Inc.

Invertebrate Acute Toxicity

Test Substance:	Alcohol C7 - 9 branched
CAS No.	68526-83-0
Method/Guideline:	US EPA 660/3-75-009
Type (test type):	Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians
GLP:	Unknown
Year (study performed):	1980
Species:	Water Flea (*Daphnia magna* Straus)
Analytical Monitoring:	No
Exposure Period:	48 hour
Statistical Method:	Spearman-Karber (Finney, D.J., 1971)
Test Conditions: • **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**	Individual treatments were prepared by adding varying amounts of test material directly to 250 mL of dilution water in glass beakers. Nominal test concentrations were 10, 18, 32, 56, 100 and 180 mg/L. Four replicates were prepared for each treatment and control. Five daphnids per replicate chamber. Test placed in a temperature-controlled waterbath at 20.5 to 21.0 Deg. C. The test was performed under static conditions. Lighting was 16 hours light : 8 hours dark. Dissolved oxygen ranged from 8.6 to 9.6 mg/L during the study. The pH was ranged from 7.8 to 8.4 during the study. Dilution water hardness was 240 mg/L as $CaCO_3$, alkalinity was 145 mg/L as $CaCO_3$, and conductivity was 600 µmhos/cm. Organisms were supplied by in-house cultures. Age = <20 hours old.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	48-hour LC50 = 31.8 mg/L (CI 26.5 - 38.2) as Total Carbon, based upon nominal concentrations.

Results continued

Nominal Conc.	% Mortality @ 48 hr.
Control	0
10 mg/L	10
18 mg/L	20
32 mg/L	25
56 mg/L	95
100 mg/L	100
180 mg/L	100

Conclusion: Test substance is considered to have moderate acute toxicity.

Reliability: Code 2, Reliable with Restrictions

Analytical verification not performed, quality assurance unknown.

Reference: Union Carbide Corp. (1980). "The Acute Toxicity of MRD-80-4 to the Water Flea (*Daphnia magna* Straus). Unpublished report.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Biodegradation

Test Substance: Alcohols C7-9, branched

CAS No. 68526-83-0

Method/Guideline: OECD 301F, 1992

Type (test type): Manometric Respirometry Test

GLP: Yes

Year (study performed): 1997

Inoculum: Domestic activated sludge

Exposure Period: 28 days

Test Conditions:

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).
Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.
Test material was tested in triplicate, controls and blanks were tested in duplicate.
Test material concentration was approximately 51 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.
Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Test material was readily biodegradable. Half-life was reached by day 11. By day 28, 82% degradation of the test material was observed. 10% biodegradation was achieved on day 3.
By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.
Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	84.7, 77.1, 84.0	82.0
Na Benzoate	91.3, 81.3	86.3

* replicate data

Conclusion: Test substance is considered readily biodegradable.

Reliability: Code 1, Reliable without Restrictions

Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 114794A..
Other (**source**):	ExxonMobil Biomedical Sciences, Inc.

Partition Coefficient

Test Substance:	Alcohol C7-9, branched
CAS No.	68526-83-0
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	2.9 - 3.4
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4. Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3. The pH of the evaluated solutions was the same as the reference solution it was evaluated against. The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	The test substance eluted as several groups. The three major components C7, C8, C9 alcohols had Log Pow values of 2.9, 3.0, and 3.4 respectively. The retention time for the 3 major components were 5.72, 6.03, and 7.28 minutes. All values were measured using High Performance Liquid Chromatography (HPLC).
Conclusion:	

Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (**source**):	ExxonMobil Biomedical Sciences, Inc.

Fish Acute Toxicity

Test Substance:	Alcohol C8 - 10 iso, C9 rich
CAS No.	68526-84-1
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1995
Species:	Rainbow Trout (*Oncorhynchus mykiss*)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Bionomial Method
Test Conditions: • **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution. Test temperature was 15.0 Deg C., Lighting was 16 hours light : 8 hours dark with 572 to 573 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.4 to 9.0 mg/L and from 4.8 to 6.3 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.8 to 8.5 during the study. Fish were not fed during the study. Fish Mean Wt.= 0.361g. Mean Total length = 3.8cm, Test Loading = 0.40 g of fish/L.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	LC50 = 10.1mg/L (CI 7.3 to 14.1), based upon measured concentrations of mean of old and new samples. Analytical method used was GC-FID LL50 = 11.2 mg/L (CI 7.5 to 16.6), based upon nominal loading levels.

Results continued

Nominal Conc.	Measured Conc.	% Mortality @ 96 hr.
Control	Below detection	0
0.7 mg/L	1.7 mg/L	0
1.5 mg/L	1.9 mg/L	0
3.3 mg/L	3.9 mg/L	0
7.5 mg/L	7.3 mg/L	0
16.6 mg/L	14.1 mg/L	100

Dissolved oxygen levels dropped below 60% of saturation in some of the treatments on Days 1 through 4 of the test. Since no mortality occurred in these treatments, the deviations are not believed to have affected the outcome of the study.

Conclusion: Test substance is considered to have moderate acute toxicity

Reliability: Code 1, Reliable without Restrictions

Reference: Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 114858.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Invertebrate Acute Toxicity

Test Substance:	Alcohol C8-10 iso, C9 rich
CAS No.	68526-84-1
Method/Guideline:	OECD 202 Daphnia sp. Acute Immobilization Test
Type (test type):	Daphnid Acute Toxicity Test
GLP:	Yes
Year (study performed):	1996
Species:	Water Flea (*Daphnia magna*)
Analytical Monitoring:	Yes
Exposure Period:	48 hour
Statistical Method:	Probit procedure of SAS (Finney, 1971)
Test Conditions: • Note: **Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**	Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added to 2.0L of dilution water in a 2L glass aspirator bottle. The solutions were mixed for 25 hours at a vortex of </= 20% of the total depth. The test solutions were removed through the outlet at the bottom of each mixing vessel into four replicates of 140 mL in 125 mL glass erlenmeyer flasks (no headspace). Five daphnids were added to each test replicate and the replicates sealed. The test was performed under static conditions with no aeration. Test temperature was 21.4 Deg C., Lighting was 16 hours light : 8 hours dark with 638 to 639 Lux during full daylight periods. Dissolved oxygen ranged from 7.3 to 8.2 mg/L during the study. The pH was ranged from 7.7 to 8.4 during the study. Organisms were supplied by in-house cultures. Age = <24 hours old, from 13 and 16-day old parents.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	48-hour EC50 = 4.9 mg/L (CI 4.5 - 5.4), based upon measured concentrations of mean of old and new samples. Analytical method used was Total Organic Carbon (TOC).

	Nominal Conc.	Measured Conc.	% Immobilization @ 24 hr.
Results continued	Control	0	0
	1.56 mg/L	0.80 mg/L	0
	3.12 mg/L	1.82 mg/L	0
	6.25 mg/L	3.05 mg/L	0
	12.5 mg/L	4.39 mg/L	40
	25.0 mg/L	6.14 mg/L	85

Conclusion: Test substance is considered to have moderate acute toxicity

Reliability: Code 1, Reliable without Restrictions

Reference: Exxon Biomedical Sciences, Inc. Acute Toxicity for Daphnia, 149542.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Algal Toxicity

Test Substance:	Alcohol C8-10 iso, C9 rich
CAS No.	68526-84-1
Method/Guideline:	7-Day Cell Multiplication Inhibition Test
Type (test type):	Static Toxicity Test
GLP:	No Data
Year (study performed):	No Data
Species/Strain:	Green Alga (*Scenedesmus quadricauda*)
Analytical Monitoring:	No
Exposure Period:	7 days
Statistical Method:	None applied. The toxicity threshold (TT) was determined graphically by plotting the highest non-toxic concentration versus its mean extinction value against the lowest toxic concentration versus its mean extinction value and calculating the toxicant concentration at 3% below the no effect level.
Test Conditions: • Note: **Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organism culture, age.**	Treatment solutions were prepared by diluting a stock isooctanol solution. Testing was conducted in metal capped, 300 ml Erlenmeyer flasks containing 50 ml of treatment solution. Treatment solutions contained isooctanol, cells, double distilled water, and a sterile, defined nutrient medium. The control solution contained nutrient medium, to which sterile double distilled water was added. Growth inhibition measurements were only determined on day 7. Cell growth was determined by using a turbidimetric procedure that measured primary light extinction (monochromatic radiation at 578 nm) through a cell suspension of 10 mm thickness.
Results: **Units/Value:** **Measurement (cells/growth)** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	7-day TT (toxicity threshold) for growth = 8.5 mg/L based on nominal values The TT value for growth is calculated by identifying the treatment level that is greater or equal to 3% below the treatment level that did not exhibit toxic effects as measured by the extinction of primary light of monochromatic radiation at 578 nm.

Conclusion:

Reliability:	(2) Reliable with restrictions Although a non-standardized method was described in the article, data were not provided on the test parameters, replication, or results from individual treatment and control solutions. This lack of information supports a reliability rating of 2.
Reference:	Bringmann, G. and R. Kuhn. 1980. Comparison of the Toxicity Thresholds of Water Pollutants to Bacteria, Algae, and Protozoa in the Cell Multiplication Inhibition Test. Water Research. 14:231-241.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Partition Coefficient

Test Substance:	Alcohol C8-10 iso, C9 rich
CAS No.	68526-84-1
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	3.4 - 3.9
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4. Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3. The pH of the evaluated solutions was the same as the reference solution it was evaluated against. The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	The test substance eluted as several groups. The three major components C8, C9, C10 alcohols had Log Pow values of 3.4, 3.8, and 3.9 respectively. The retention time for the 3 major components were 6.91, 8.42, and 8.96 minutes. All values were measured using High Performance Liquid Chromatography (HPLC).
Conclusion:	

Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (**source**):	ExxonMobil Biomedical Sciences, Inc.

Fish Acute Toxicity

Test Substance:	Alcohol C9 - 11 iso, C10 rich
CAS No.	68526-85-2
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1995
Species:	Rainbow Trout (*Oncorhynchus mykiss*)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Probit procedure of SAS (Finney, 1971)
Test Conditions: • Note: **Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19.5L of dilution water in a 20L glass carboy. The carboys were covered with an opaque covering to prevent photochemical degradation of the soluble components. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution. Test temperature was 15.0 Deg C., Lighting was 16 hours light : 8 hours dark with 569 to 572 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.4 to 9.9 mg/L and from 5.7 to 7.6 mg/L in "old" solutions prior to renewals. The pH was ranged from 7.0 to 8.5 during the study. Fish were not fed during the study. Fish Mean Wt.= 0.185g. Mean Total length = 3.0cm, Test Loading = 0.21 g of fish/L.
Results: **Units/Value:** • Note: **Deviations from protocol or guideline, analytical method, biological observations, control survival.**	LC50 = 3.1mg/L (CI 2.4 to 4.0), based upon measured concentrations of mean of old and new samples. Analytical method used was GC-FID LL50 = 3.0 mg/L (Could not calculate CI), based upon nominal loading levels.

Results continued

Nominal Conc.	Measured Conc.	% Mortality @ 96 hr.
Control	Below detection	7
1.2 mg/L	1.2 mg/L	13
2.5 mg/L	2.4 mg/L	13
5 mg/L	5.2 mg/L	100
10 mg/L	9.9 mg/L	100
20 mg/L	19.5 mg/L	100

Dissolved oxygen levels dropped below 60% (57%)of saturation in the 2.4 mg/L treatment on Days 3 and 4 of the test. Since only 13% mortality occurred at this level, and the solutions were renewed daily, this drop in DO did not affect the outcome of the study.

Conclusion: Test substance is considered to have moderate acute toxicity

Reliability: Code 1, Reliable without Restrictions

Reference: Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 114958.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Biodegradation

Test Substance: Alcohol C9 - 11 iso, C10 rich

CAS No. 68526-85-2

Method/Guideline: OECD 301F, 1992

Type (test type): Manometric Respirometry Test

GLP: Yes

Year (study performed): 1997

Inoculum: Domestic activated sludge

Exposure Period: 28 days

Test Conditions:

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).
Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.
Test material was tested in triplicate, controls and blanks were tested in duplicate.
Test material concentration was approximately 43 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.
Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Test material was readily biodegradable. Half-life was reached by day 11. By day 28, 71.1% degradation of the test material was observed. 10% biodegradation was achieved on day 4.
By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.
Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	74.0, 72.6, 66.5	71.1
Na Benzoate	91.3, 81.3	86.3

* replicate data

Conclusion: Test substance is considered readily biodegradable.

Reliability: Code 1, Reliable without Restrictions

Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 114994A..
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Partition Coefficient

Test Substance:	Alcohol C9 - 11 iso, C10 rich
CAS No.	68526-85-2
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	3.8
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4. Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3. The pH of the evaluated solutions was the same as the reference solution it was evaluated against. The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	The test substance eluted as several groups. The two major components C9, C10 alcohols had Log Pow values of 3.8. The retention time for the 2 major components were 8.37, and 8.74 minutes. All values were measured using High Performance Liquid Chromatography (HPLC).
Conclusion:	

Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Water Solubility

Test Substance:	Alcohol C9-11, iso, C10 rich
CAS No.	68526-85-2
Method/Guideline:	No data (No standard guidelines are available for this method)
Year (guideline):	No data
Type (test type):	Water Solubility (Slow Stir Method)
GLP:	No
Year (study **performed):**	1999
Temperature:	20 Deg C
pH value:	No data
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Test and control systems were established at 20 Deg. C in a laboratory incubator. The test systems consisted of a glass aspirator bottle containing 2L of glass-distilled water (gdH_2O) and a 4cm-glass stir bar. Prior to use, the aspirator bottle was rinsed with a mixture of residue grade methylene chloride:acetone (1:1) and issoctane and then allowed to dry in a laboratory fume hood. The bottles were rinsed three times with gdH_2O before being filled for the test. The control and test vessels were poisoned with 50 mg/L mercuric chloride ($HgCl_2$). The test vessel was prepared at a loading of ~100 mg/L by adding the neat test substance to the surface of the water. The systems were stirred quiescently so that there was little, if any, visible vortex. The analytical samples were removed from the solution (through the outlet at the bottom of the vessel) into a volatile organic analysis sample vial and refrigerated until analyzed. Prior to analysis, aliquots were transferred to headspace sample vials.
Results: Units/Value: • Note: **Deviations from protocol or guideline, analytical method.**	Water solubility = 75 mg/L. Samples measured over 21 equilibration days on triplicate analyses. Day 1 = 50.9 mg/L Day 3 = 66.6 mg/L Day 7 = 75.0 mg/L Day 21 = 73.9 mg/L The clear aqueous solution was analytically measured by gas chromatography using mass selective detection (GC-MSD) in the selective ion monitoring mode.

Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1999. Study 118538, Water Solubility Test.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Fish Acute Toxicity

Test Substance:	Alcohol C11 - 14 iso, C12 rich
CAS No.	68526-86-3
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1997
Species:	Rainbow Trout (*Oncorhynchus mykiss*)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Probit procedure of SAS (Finney, 1971)
Test Conditions: • **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution. Test temperature was 15.1 Deg C., Lighting was 16 hours light : 8 hours dark with 749 to 752 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.5 to 9.8 mg/L and from 3.9 to 8.0 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.6 to 8.1 during the study. Fish were not fed during the study. Fish Mean Wt.= 0.623g. Mean Total length = 4.3cm, Test Loading = 0.69 g of fish/L.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	LC50 = 1.2 mg/L (CI 0.98 to 1.4), based upon measured concentrations of mean of old and new samples. Analytical method used was GC-MSD LL50 = 1.7 mg/L (CI 1.4 to 3.3), based upon nominal loading levels.

Results continued

Nominal Conc.	Measured Conc.	% Mortality @ 96 hr.
Control	Below detection	0
0.4 mg/L	0.22 mg/L	0
0.75 mg/L	0.43 mg/L	7
1.5 mg/L	1.13 mg/L	33
3.0 mg/L	1.18 mg/L	100
6.0 mg/L	1.78 mg/L	100

Dissolved oxygen levels dropped below 60% (40-60%) of saturation in some of the treatments on Days 1 through 4 of the test. Based on mortality observations, these deviations are not believed to have affected the outcome of the study.

Conclusion: Test substance is considered to have moderate acute toxicity

Reliability: Code 1, Reliable without Restrictions

Reference: Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 118558.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Invertebrate Acute Toxicity

Test Substance:	Alcohol C11 - 14 iso, C12 rich
CAS No.	68526-86-3
Method/Guideline:	OECD 202 Daphnia sp. Acute Immobilization Test
Type (test type):	Daphnid Acute Toxicity Test
GLP:	Yes
Year (study performed):	1997
Species:	Water Flea (*Daphnia magna*)
Analytical Monitoring:	Yes
Exposure Period:	24 hour
Statistical Method:	Probit procedure of SAS (Finney, 1971)
Test Conditions: • Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.	Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 2.0L of dilution water in a 2L glass aspirator bottle. The solutions were mixed for 23 hours at a vortex of </= 10% of the total depth. The test solutions were removed through the outlet at the bottom of each mixing vessel into four replicates of 140 mL in 125 mL glass erlenmeyer flasks (no headspace). Five daphnids were added to each test replicate and the replicates sealed. The test was performed under static conditions with no aeration. Test temperature was 19.8 Deg C., Lighting was 16 hours light : 8 hours dark with 443 to 577 Lux during full daylight periods. Dissolved oxygen ranged from 8.0 to 8.5 mg/L during the study. The pH was ranged from 7.0 to 7.6 during the study. Organisms were supplied by in-house cultures. Age = <24 hours old
Results: Units/Value:	24-hour EC50 = 0.81 mg/L (Could not calculate CI), based upon measured concentrations of mean of old and new samples.
• Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	Analytical method used was GC-MSD

Results continued

Nominal Conc.	Measured Conc.	% Immobilization @ 24 hr.
Control	Below detection	0
0.31 mg/L	0.45 mg/L	25
0.63 mg/L	1.14 mg/L	85
1.25 mg/L	1.75 mg/L	100
2.5 mg/L	2.3 mg/L	95
5.0 mg/L	2.5 mg/L	100

Conclusion: The results of this study confirm the EC50 is below 1.0 mg/L

Reliability: Code 1, Reliable without Restrictions

Reference: Exxon Biomedical Sciences, Inc. Acute Toxicity for Daphnia, 118542.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Biodegradation

Test Substance:	Alcohol C11 - 14 iso, C12 rich
CAS No.	68526-86-3
Method/Guideline:	OECD 301F, 1992
Type (test type):	Manometric Respirometry Test
GLP:	Yes
Year (study performed):	1997
Inoculum:	Domestic activated sludge
Exposure Period:	28 days
Test Conditions: • Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.	Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride). Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test material was tested in triplicate, controls and blanks were tested in duplicate. Test material concentration was approximately 43 mg/L. Sodium benzoate (positive control) concentration was 50mg/L. Test temperature was 22 +/- 1 Deg C. All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
Results: Units/Value: • Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	Test material was not readily biodegradable. Half-life was reached by day 21. By day 28, 59.6% degradation of the test material was observed. 10% biodegradation was achieved on day 8. By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	56.5, 60.3, 61.8	59.6
Na Benzoate	92.5, 92.7	92.6

* replicate data

Conclusion:	Test substance is considered not readily biodegradable.
Reliability:	Code 1, Reliable without Restrictions

Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 195994A..
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Partition Coefficient

Test Substance:	Alcohol C11 - 14 iso, C12 rich
CAS No.	68526-86-3
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	4.2 - 4.8
Test Conditions: • Note: Concentration prep., vessel type, replication, test conditions.	The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4. Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3. The pH of the evaluated solutions was the same as the reference solution it was evaluated against. The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.
Results: Units/Value: • Note: Deviations from protocol or guideline, analytical method.	The test substance eluted as several groups. The four major components C9, C10, C11, C12 alcohols had Log Pow values of 4.2, 4.5, 4.7, and 4.8 respectively. The retention time for the 4 major components were 11.13, 13.36, 14.75, and 16.66 minutes. All values were measured using High Performance Liquid Chromatography (HPLC).
Conclusion:	

Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Fish Acute Toxicity

Test Substance:	Alcohol C11 - 14 iso, C13 rich
CAS No.	68526-86-3
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1998
Species:	Rainbow Trout (*Oncorhynchus mykiss*)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Spearman-Karber Method (Hamilton, et al, 1977)
Test Conditions: • **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution. Test temperature was 13.8 Deg C., Lighting was 16 hours light : 8 hours dark with 551 to 736 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.3 to 9.2 mg/L and from 6.6 to 8.8 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.6 to 8.2 during the study. Fish were not fed during the study. Fish Mean Wt.= 0.131g. Mean Total length = 2.7cm, Test Loading = 0.15 g of fish/L.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	LC50 = 0.42 mg/L (CI 0.37 to 0.48), based upon measured concentrations of mean of old and new samples. Analytical method used was GC-MSD LL50 = 0.64 mg/L (CI 0.57 to 0.73), based upon nominal loading levels.

survival.

Results continued

Nominal Conc.	Measured Conc.	% Mortality @ 96 hr.
Control	Below detection	0
0.25 mg/L	0.17 mg/L	0
0.5 mg/L	0.32 mg/L	13
1.0 mg/L	0.67 mg/L	100
2.0 mg/L	0.94 mg/L	100
5.0 mg/L	0.93 mg/L	100

Conclusion: Test substance is considered to have high acute toxicity

Reliability: Code 1, Reliable without Restrictions

Reference: Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 118358A.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Invertebrate Acute Toxicity

Test Substance:	Alcohol C11 - 14 iso, C13 rich
CAS No.	68526-86-3
Method/Guideline:	US EPA TSCA 797.1300
Type (**test type**):	Daphnid Acute Toxicity Test
GLP:	Unknown
Year (study performed):	1986
Species:	Water Flea (*Daphnia magna*)
Analytical **Monitoring:**	Yes
Exposure Period:	48 hour
Statistical Method:	Probit procedure based on Litchfield-Wilcoxon (1949)
Test Conditions: • **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions,** organisms **supplier, age, size,** loading.	The water soluble fraction (WSF) was prepared by combining the test substance with dilution water at a ratio of 1:150. The solutions were mixed for 96 hours and allowed to settle for 1 hour prior to use as the 100% WSF stock solution. Test solutions were prepared by diluting the 100% WSF stock. Two replicates of 250 mL in 400 mL autoclaved glass beakers were prepared at each treatment level. Ten daphnids per replicate chamber. Test chambers were covered with glass and placed in a temperature-controlled waterbath. The test was performed under static conditions. Test temperature was 20.8 Deg C., Lighting was 16 hours light : 8 hours dark with 57.5 to 67.3 footcandles during full daylight periods. Dissolved oxygen ranged from 8.1 to 9.1 mg/L during the study. The pH was ranged from 7.8 to 8.2 during the study. Dilution water hardness was 130 mg/L as $CaCO_3$. Organisms were supplied by in-house cultures. Age = <24 hours old from 19-day old parents.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	48-hour LC50 = 0.71 mg/L (CI 0.59 - 0.85) as Total Carbon, based upon mean measured concentrations of Day 0 and Day 2 samples. 48-hour LC50 value equivalent to 16.7% WSF. Analytical method used was Total Carbon

Results continued

Nominal Conc.	Measured Conc.	% Mortality @ 48 hr.
Control	-	0
6.25% WSF	0.28 mg/L	0
12.5% WSF	0.58 mg/L	30
25% WSF	1.03 mg/L	85
50% WSF	1.85 mg/L	100
100% WSF	4.17 mg/L	100

Conclusion: Test substance is considered to have high acute toxicity.

Reliability: Code 2, Reliable with Restrictions

Analytical verification not test substance specific, quality assurance unknown.

Reference: Exxon Biomedical Sciences, Inc. Static Acute Daphnia Toxicity Test, 269342.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Biodegradation

Test Substance: Alcohol C11 - 14 iso, C13 rich

CAS No. 68526-86-3

Method/Guideline: OECD 301F, 1992

Type (**test type**): Manometric Respirometry Test

GLP: Yes

Year (study performed): 1998

Inoculum: Domestic activated sludge

Exposure Period: 28 days

Test Conditions:

- Note: **Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).
Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.
Test material was tested in triplicate, controls and blanks were tested in duplicate.
Test material concentration was approximately 57 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.
Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Test material was not readily biodegradable. Half-life was reached by day 25. By day 28, 58.1% degradation of the test material was observed. 10% biodegradation was achieved on day 7.
By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.
Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	60.1, 60.7, 53.7	58.1
Na Benzoate	87.1, 85.4	86.2

* replicate data

Conclusion: Test substance is considered not readily biodegradable.

Reliability: Code 1, Reliable without Restrictions

Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 180294A..
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Partition Coefficient

Test Substance:	Alcohol C11 - 14 iso, C13 rich
CAS No.	68526-86-3
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	4.2 - 5.0
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4. Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3. The pH of the evaluated solutions was the same as the reference solution it was evaluated against. The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	The test substance eluted as several groups. The five major components C9, C10, C11, C12, C13 alcohols had Log Pow values of 4.2, 4.4, 4.5, 4.7, and 5.0 respectively. The retention time for the 4 major components were 11.04, 12.02, 13.53, 14.69, and 18.40 minutes. All values were measured using High Performance Liquid Chromatography (HPLC).
Conclusion:	

Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Water Solubility

Test Substance:	Alcohol C11-14, iso, C13 rich
CAS No.	68526-86-3
Method/Guideline:	No data (No standard guidelines are available for this method)
Year (guideline):	No data
Type (test type):	Water Solubility (Slow Stir Method)
GLP:	No
Year (study performed):	1999
Temperature:	20 Deg C
pH value:	No data
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Test and control systems were established at 20 Deg. C in a laboratory incubator. The test systems consisted of a glass aspirator bottle containing 2L of glass-distilled water (gdH_2O) and a 4cm-glass stir bar. Prior to use, the aspirator bottle was rinsed with a mixture of residue grade methylene chloride:acetone (1:1) and issoctane and then allowed to dry in a laboratory fume hood. The bottles were rinsed three times with gdH_2O before being filled for the test. The control and test vessels were poisoned with 50 mg/L mercuric chloride ($HgCl_2$). The test vessel was prepared at a loading of ~100 mg/L by adding the neat test substance to the surface of the water. The systems were stirred quiescently so that there was little, if any, visible vortex. The analytical samples were removed from the solution (through the outlet at the bottom of the vessel) into a volatile organic analysis sample vial and refrigerated until analyzed. Prior to analysis, aliquots were transferred to headspace sample vials.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Water solubility = 5.8 mg/L. Samples measured over 21 equilibration days on triplicate analyses. Day 1 = 3.09 mg/L Day 3 = 5.19 mg/L Day 7 = 5.79 mg/L Day 21 = 5.38 mg/L The clear aqueous solution was analytically measured by gas chromatography using mass selective detection (GC-MSD) in the selective ion monitoring mode.

Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1999. Study 118538, Water Solubility Test.
Other (**source**):	ExxonMobil Biomedical Sciences, Inc.

IUCLID

Data Set

Existing Chemical	:	ID: 104-76-7
CAS No.	:	104-76-7
EINECS Name	:	2-ethylhexan-1-ol
EINECS No.	:	203-234-3
TSCA Name	:	1-Hexanol, 2-ethyl-
Molecular Formula	:	C8H18O

Producer Related Part

Company	:	EUROPEAN COMMISSION - European Chemicals Bureau
Creation date	:	10.02.2000

Substance Related Part

Company	:	EUROPEAN COMMISSION - European Chemicals Bureau
Creation date	:	10.02.2000
Memo	:	
Printing date	:	05.11.2001
Revision date	:	10.02.2000
Date of last Update	:	10.02.2000
Number of Pages	:	163
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	
Name	:	Alusuisse Italia Spa
Partner	:	
Date	:	
Street	:	via del Pruneto, 40
Town	:	I-52027 S.Giovanni Valdarno (AR)
Country	:	Italy
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential

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

Type	:	
Name	:	Atochem
Partner	:	
Date	:	
Street	:	
Town	:	92080 Paris la Defense
Country	:	France
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential

Type	:	
Name	:	Atochem
Partner	:	
Date	:	
Street	:	4, Cours Michelet
Town	:	92080 Paris la Defense
Country	:	France
Phone	:	
Telefax	:	

Telex	:	
Cedex	:	
Type	:	
Name	:	BASF AG
Partner	:	
Date	:	
Street	:	Karl-Bosch-Str
Town	:	67056 Ludwigshafen
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential
Type	:	
Name	:	BASF AG
Partner	:	
Date	:	
Street	:	Karl-Bosch-Str
Town	:	67056 Ludwigshafen
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Type	:	
Name	:	BASF Espanola S. A.
Partner	:	
Date	:	
Street	:	
Town	:	43080 Tarragona
Country	:	Spain
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential
Type	:	
Name	:	BASF Espanola S. A.
Partner	:	
Date	:	
Street	:	
Town	:	43080 Tarragona
Country	:	Spain
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Type	:	
Name	:	BP Chemicals Ltd.
Partner	:	
Date	:	
Street	:	Belgrave House, 76 Buckingham Palace Road
Town	:	SW1 WOSU London
Country	:	United Kingdom
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential

Type	:	
Name	:	BP Chemicals Ltd.
Partner	:	
Date	:	
Street	:	76, Buckingham Palace Road
Town	:	SW1 WOSU London
Country	:	United Kingdom
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Type	:	
Name	:	BUNA GMBH
Partner	:	
Date	:	
Street	:	Sparte Organica Bau G59
Town	:	06258 Schkopau
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential

Type	:	
Name	:	BUNA GMBH
Partner	:	
Date	:	
Street	:	Sparte Organica Bau G59
Town	:	06258 Schkopau
Country	:	Germany
Phone	:	03461 49 2007
Telefax	:	03461 49 2670
Telex	:	
Cedex	:	

Type :

Name	:	Celanese GmbH
Partner	:	
Date	:	
Street	:	Industriepark Höchst
Town	:	65926 Frankfurt am Main
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Type	:	
Name	:	Ciba-Geigy SpA
Partner	:	
Date	:	
Street	:	S.S.233 Km 20.5 Varesina
Town	:	I-21047 Saronno(VA)
Country	:	Italy
Phone	:	39 2 96541
Telefax	:	39 2 96701091
Telex	:	
Cedex	:	

Type	:	
Name	:	CYTEC INDUSTRIES B.V.
Partner	:	
Date	:	
Street	:	P.O.Box 5195 , Botlekweg 175
Town	:	3197 ZH Rotterdam
Country	:	Netherlands
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Type	:	
Name	:	ECEM European Chemical Marketing B.V.
Partner	:	
Date	:	
Street	:	Hogehilweg 10
Town	:	1101 CC Amsterdam
Country	:	Netherlands
Phone	:	020-6912001
Telefax	:	020-6911930
Telex	:	
Cedex	:	

Type	:	
Name	:	Helm AG
Partner	:	
Date	:	
Street	:	Nordkanalstrasse 28
Town	:	20097 Hamburg
Country	:	Germany
Phone	:	+49402375-0
Telefax	:	+49402375-90
Telex	:	2170150
Cedex	:	

Type	:	
Name	:	Hoechst AG
Partner	:	

Date	:	
Street	:	
Town	:	65903 Frankfurt/Main
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential

Type	:	
Name	:	Hoechst AG
Partner	:	
Date	:	
Street	:	Postfach 80 03 20 Brüningstrasse 50
Town	:	65903 Frankfurt/Main
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Type	:	
Name	:	Huels AG
Partner	:	
Date	:	
Street	:	Postfach
Town	:	45764 Marl
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential

Type	:	
Name	:	Huels AG
Partner	:	
Date	:	
Street	:	Postfach
Town	:	D-45764 Marl
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Type	:	
Name	:	International Speciality Chemicals Ltd.
Partner	:	
Date	:	
Street	:	Charleston Industries Estate, Hardley, Hythe

Town	:	SO45 32G Southampton
Country	:	United Kingdom
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Type	:	
Name	:	Lubrizol Great Britain Limited
Partner	:	
Date	:	
Street	:	P.O.Box 88
Town	:	DE56 1QN Belper, Derby
Country	:	United Kingdom
Phone	:	332-842211
Telefax	:	332-842303
Telex	:	37445
Cedex	:	
Type	:	
Name	:	Neste Oxo AB
Partner	:	
Date	:	
Street	:	
Town	:	444 84 Stenungsund
Country	:	Sweden
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential
Type	:	
Name	:	Neste Oxo AB
Partner	:	
Date	:	
Street	:	
Town	:	44484 Stenungsund
Country	:	Sweden
Phone	:	+46 303 85600
Telefax	:	+46 303 856 07
Telex	:	27052 nestox S
Cedex	:	
Type	:	
Name	:	Petrasol B.V.
Partner	:	
Date	:	
Street	:	P.O.Box 222
Town	:	4200 AE Gorinchem
Country	:	Netherlands
Phone	:	+31 183 630555
Telefax	:	+31 183 632272
Telex	:	23602 petr nl
Cedex	:	
Type	:	

Name	:	Vinyl Additives GmbH formerly CIBA Additive GmbH
Partner	:	
Date	:	
Street	:	Chemiestrasse
Town	:	D-68623 Lampertheim
Country	:	Germany
Phone	:	+49(6206)15-0
Telefax	:	+49(6206)152511
Telex	:	
Cedex	:	

Type	:	
Name	:	VOS B.V.
Partner	:	
Date	:	
Street	:	Ondernemingsweg 1A
Town	:	2404 HM Alphen aan den Rijn
Country	:	Netherlands
Phone	:	31-172-431601
Telefax	:	31-172-432494
Telex	:	
Cedex	:	

1.0.2 LOCATION OF PRODUCTION SITE

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

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

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

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

1-Ethyl-1-hexanol

Source	:	Neste Oxo AB Stenungsund
		Neste Oxo AB Stenungsund
		ECB - Existing Chemicals Ispra (VA)
		Hoechst AG Frankfurt/Main
		Neste Oxo AB Stenungsund
		ECB - Existing Chemicals Ispra (VA)
		Hoechst AG Frankfurt/Main
		Celanese GmbH Frankfurt am Main

1-Hexanol, 2-ethyl-
Source : Huels AG Marl

1-Hexanol, 2-ethyl- (8Cl, 9Cl)
Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-EH
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethyl-1-hexanol
Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-ethyl-1-hexanol
Remark : Also known as:
2-ethylhexyl alcohol
2-EH
Iso-octanol
Source : International Speciality Chemicals Ltd. Southampton

2-Ethylhexaan-1-ol
Source : VOS B.V. Alphen aan den Rijn

2-Ethylhexanol
Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Neste Oxo AB Stenungsund
Hoechst AG Frankfurt/Main
Huels AG Marl
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Vinyl Additives GmbH formerly CIBA Additive GmbH Lampertheim

2-Ethylhexanol iso-Octanol
Source : BUNA GMBH Schkopau
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
BUNA GMBH Schkopau
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Celanese GmbH Frankfurt am Main

2-Ethylhexanol-1
Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexanol; 2-Ethylhexylalcohol; Isooctanol; Octylalcohol; 2-EH
Source : Atochem Paris la Defense
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexanol; ethylhexanol
Source : ISIS/RISKLINE release VI, 1997, Haskoning
Petrasol B.V. Gorinchem

2-Ethylhexyl alcohol
Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Neste Oxo AB Stenungsund
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexylalkohol
Source : Huels AG Marl
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Huels AG Marl
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Etil esanolo
Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2EH
Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)

alcol 2-etilesilico
Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)

ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Ethylhexanol
Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Neste Oxo AB Stenungsund
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Isooctanol
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Huels AG Marl
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

isoottanolo
Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Octyl alcohol
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

1.3 IMPURITIES

1.4 ADDITIVES

1.5 QUANTITY

Production during the last 12 months :
Import during the last 12 months :
Quantity : 500 000 - 1 000 000 tonnes in

Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential
Production during the last 12 months	:	
Import during the last 12 months	:	
Quantity	:	more than 1 000 000 tonnes in

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.7 USE PATTERN

Type	:	type
Category	:	Non dispersive use
Type	:	type
Category	:	Use in closed system
Type	:	type
Category	:	Wide dispersive use
Type	:	industrial
Category	:	Basic industry: basic chemicals
Type	:	industrial
Category	:	Chemical industry: used in synthesis
Type	:	industrial
Category	:	Paints, lacquers and varnishes industry
Type	:	industrial
Category	:	Polymers industry
Type	:	industrial
Category	:	Textile processing industry
Type	:	industrial
Category	:	other
Type	:	use
Category	:	Fuel additives
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main
Flag	:	non confidential
Type	:	use
Category	:	Fuel additives
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

Flag	:	non confidential
Type	:	use
Category	:	Fuel additives
Type	:	use
Category	:	Intermediates
Type	:	use
Category	:	Lubricants and additives
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main
Flag	:	non confidential
Type	:	use
Category	:	Lubricants and additives
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential
Type	:	use
Category	:	Lubricants and additives
Type	:	use
Category	:	Softeners
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential
Type	:	use
Category	:	Softeners
Type	:	use
Category	:	Solvents
Type	:	use
Category	:	other

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit	:	MAK (DE)
Limit value	:	
Remark	:	Kein MAK-Wert festgelegt
Source	:	BASF AG Ludwigshafen BASF Espanola S. A. Tarragona BASF AG Ludwigshafen BASF Espanola S. A. Tarragona ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main BASF AG Ludwigshafen BASF Espanola S. A. Tarragona ECB - Existing Chemicals Ispra (VA)

Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(1)

Type of limit	:	MAK (DE)
Limit value	:	
Country	:	Germany
Remark	:	MAK not established.
Source	:	Huels AG Marl

(2)

Type of limit	:	OES (UK)
Limit value	:	271 mg/m3
Short term exposure		
Limit value	:	
Schedule	:	8 hour(s)
Frequency	:	times
Remark	:	UK OES not assigned specifically. Figure quoted is for Iso-octyl alcohol (mixed isomers) - from EH40 1998 edition.
Source	:	International Speciality Chemicals Ltd. Southampton

Type of limit	:	TLV (US)
Limit value	:	250 mg/m3
Source	:	Alusuisse Italia Spa S.Giovanni Valdarno (AR) Alusuisse Italia Spa S.Giovanni Valdarno (AR) ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Alusuisse Italia Spa S.Giovanni Valdarno (AR) ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Remark	:	No data on Occupational Exposure Limit Value.
Source	:	Atochem Paris la Defense
Remark	:	No Occupational Exposure Limit available.
Source	:	Neste Oxo AB Stenungsund

1.9 SOURCE OF EXPOSURE

Remark : PROFESSIONAL/OCCUPATIONAL EXPOSURE DURING PRODUCTION

Process description

1. Production of "oxo alcohols" (2-ethylhexanol, normal and iso-butanol) is performed through several steps of continuous and closed chemical processes.
The first step is the production of synthesis gas obtained by partial oxidation of natural gas.
This so called syngas is used to hydroformylate propylene, a reaction which produces a mixture of n- and isobutyraldehyde.

- 2-Ethylhexanol production
2ethylhexanol is produced by aldolisation of normal butyraldehyde, followed by hydrogenation and distillation.
- Storage and despatch of Oxo Alcohols
Oxo alcohols are stored in closed tanks where vent gas is collected and burnt in a residual gas incinerator.
There is no equipment opening during production, hence

exposure to chemicals is quite limited.
Product despatch is done by road, rail, or ship mainly.
2. Number of sites
One production site located in Lavera, France.
3. Protective measures
Procedures and equipment used minimise personnel exposure. Workers and contractors wear gloves, safety glasses or goggies, and long sleeves clothes.
4. Industrial hygiene monitoring
Continuous on line explisimeters detect leaks.
Local explosivity analysis is made before maintenance work.
Outside operators are watching any abnormal noise or odor.
Routine analysis of hydrocarbon in atmosphere is done.
Worker have a yearly medical follow up.
COV monitoring program underway : will be finished in 18 months.

ENVIRONMENTAL EXPOSURE DURING PRODUCTION AND USE

1. Distribution pattern

Production lossed	ethyl-2-hexanol
to air	0.001 %
to water	0.004 %

2. Primary exposed environment
All spills are collected. Plant drainage is collected to chemical water sewer. This water is treated in a water treatment plant.
3. Release pattern
Point source and diffuse.

GENERAL USE PATTERN

100 % professional use.

ADDITIONAL INFORMATION

1. Indication of measured exposure levels.
Atmosphere analysis performed 2 times per year indicate an average value of 4 vpm of chemical expressed as CH4.
VOC monitoring program will allow a better follow up.

Source : Atochem Paris la Defense
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Remark : La sostanza in esame è utilizzata come materia prima nello Stabilimento Distillerie Italiane dell'Alusuisse Italia Spa, nel processo di sintesi dei plastificanti.
Il processo dove viene impiegata la sostanza 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 ecologico dello Stabilimento, quindi immessa n acque superficiali nei limiti stabiliti dalle leggi nazionali (Legge Merli n° 319/76).

I gas ricondensabili, contenenti tracce di sostanze organiche, provenienti dalle apparecchiature di processo, sono collettati e inviati al trattamento di depurazione in apposito impianto di ossidazione termica e quindi 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 - 25 Nm3/h per Ton. di sostanza
* durata emissione - continua

Fattori potenziali di esposizione umana
La sostanza ha un'alta temperatura di ebollizione ed una bassa tensione di vapore, presenta altresuna buona soglia olfattiva.Considerando che la sostanza viene utilizzata in processi a ciclo chiuso si ritiene insignificante il potenziale di esposizione ai vapori da parte dell'utilizzatore.

Settori di impiego

La sostanza fa parte della famiglia degli OXOalcoli e viene impiegata come materia prima nel processo di sintesi del plastificante che a sua volta costituisce un additivo per la produzione di materiali termoplastici a base di PVC. Nel plastificante la sostanza non si trova più allo stato libero ma come estere dell'anidride ftalica.

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

Country : Sweden

Remark : One plant in Sweden produces 2-ethylhexanol. The production units are located outdoors and the average concentration in the air is 0.02 ppm. The type of release to the air is both point source and diffuse.

The major part of produced 2-ethylhexanol is used in the production of plasticisers.

The production of 2-ethylhexanol is a closed process.

No 2-ethylhexanol is used in cosumer products.

Source : Neste Oxo AB Stenungsund

(3)

Remark : La sostanza in esame è utilizzata come materia prima nello Stabilimento Distillerie Italiane dell'Alusuisse Italia Spa, nel processo di sintesi dei plastificanti.
Il processo dove viene impiegata la sostanza 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 ecologico dello Stabilimento, quindi immessa n acque superficiali nei limiti stabiliti dalle leggi nazionali (Legge Merli n° 319/76).

I gas ricondensabili, contenenti tracce di sostanze organiche, provenienti dalle apparecchiature di processo, sono collettati e inviati al trattamento di depurazione in apposito impianto di ossidazione termica e quindi 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 - 25 Nm3/h per Ton. di sostanza
* durata emissione - continua

Fattori potenziali di esposizione umana
La sostanza ha un'alta temperatura di ebollizione ed una bassa tensione di vapore, presenta altresuna buona soglia olfattiva.Considerando che la sostanza viene utilizzata in processi a ciclo chiuso si ritiene insignificante il potenziale di esposizione ai vapori da parte dell'utilizzatore.

Settori di impiego

La sostanza fa parte della famiglia degli OXOalcoli e viene impiegata come materia prima nel processo di sintesi del

plastificante che a sua volta costituisce un additivo per la produzione di materiali termoplastici a base di PVC. Nel plastificante la sostanza non si trova più allo stato libero ma come estere dell'anidride ftalica.

Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Country : Sweden

Remark : One plant in Sweden produces 2-ethylhexanol. The production units are located outdoors and the average concentration in the air is 0.02 ppm. The type of release to the air is both point source and diffuse.

The major part of produced 2-ethylhexanol is used in the production of plasticisers.

The production of 2-ethylhexanol is a closed process.

No 2-ethylhexanol is used in cosumer products.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(3)

Remark : La sostanza in esame è utilizzata come materia prima nello Stabilimento Distillerie Italiane dell'Alusuisse Italia Spa, nel processo di sintesi dei plastificanti.
Il processo dove viene impiegata la sostanza 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 ecologico dello Stabilimento, quindi immessa n acque superficiali nei limiti stabiliti dalle leggi nazionali (Legge Merli n° 319/76).

I gas ricondensabili, contenenti tracce di sostanze organiche, provenienti dalle apparecchiature di processo, sono collettati e inviati al trattamento di depurazione in apposito impianto di ossidazione termica e quindi 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 - 25 Nm3/h per Ton. di sostanza
* durata emissione - continua

Fattori potenziali di esposizione umana
La sostanza ha un'alta temperatura di ebollizione ed una bassa tensione di vapore, presenta altresuna buona soglia olfattiva.Considerando che la sostanza viene utilizzata in processi a ciclo chiuso si ritiene insignificante il potenziale di esposizione ai vapori da parte dell'utilizzatore.

Settori di impiego

La sostanza fa parte della famiglia degli OXOalcoli e viene impiegata come materia prima nel processo di sintesi del plastificante che a sua volta costituisce un additivo per la produzione di materiali termoplastici a base di PVC. Nel plastificante la sostanza non si trova più allo stato libero ma come estere dell'anidride ftalica.

Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Country : Sweden
Remark : One plant in Sweden produces 2-ethylhexanol. The production units are located outdoors and the average concentration in the air is 0.02 ppm. The type of release to the air is both point source and diffuse.

The major part of produced 2-ethylhexanol is used in the production of plasticisers.

The production of 2-ethylhexanol is a closed process.

No 2-ethylhexanol is used in cosumer products.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(3)

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

Classified by	:	KBwS (DE)
Labelled by	:	KBwS (DE)
Class of danger	:	2 (water polluting)
Source	:	BASF AG Ludwigshafen BASF Espanola S. A. Tarragona

Classified by	:	KBwS (DE)
Labelled by	:	
Class of danger	:	2 (water polluting)
Country	:	Germany
Remark	:	Kenn-Nr. 134
Source	:	Huels AG Marl ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Huels AG Marl ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(4)

Classified by	:	KBwS (DE)
Labelled by	:	KBwS (DE)
Class of danger	:	2 (water polluting)
Country	:	Germany
Remark	:	Katalognummer 134
Source	:	Huels AG Marl

(2)

1.14.2 MAJOR ACCIDENT HAZARDS

Legislation	:	Stoerfallverordnung (DE)
Substance listed	:	no
No. in directive	:	
Source	:	BASF AG Ludwigshafen BASF Espanola S. A. Tarragona

(5)

Legislation	:	Stoerfallverordnung (DE)
Substance listed	:	no
No. in directive	:	
Source	:	Hoechst AG Frankfurt/Main

(6)

Legislation	:	Stoerfallverordnung (DE)
Substance listed	:	no
No. in directive	:	
Country	:	Germany
Remark	:	Stoerfallverordnung 1991
Source	:	Huels AG Marl

(2)

Legislation	:	Stoerfallverordnung (DE)
Substance listed	:	no

No. in directive	:	
Source	:	Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(6)

1.14.3 AIR POLLUTION

Classified by	:	TA-Luft (DE)
Labelled by	:	TA-Luft (DE)
Number	:	3.1.7 (organic substances)
Class of danger	:	III
Source	:	BASF Espanola S. A. Tarragona

(7)

Classified by	:	TA-Luft (DE)
Labelled by	:	
Number	:	3.1.7 (organic substances)
Class of danger	:	III
Remark	:	Selbsteinstufung
Source	:	Hoechst AG Frankfurt/Main

(8)

Classified by	:	TA-Luft (DE)
Labelled by	:	TA-Luft (DE)
Number	:	3.1.7 (organic substances)
Class of danger	:	III
Country	:	Germany
Remark	:	Appendix E
Source	:	Huels AG Marl

(2)

Classified by	:	TA-Luft (DE)
Labelled by	:	
Number	:	3.1.7 (organic substances)
Class of danger	:	III
Remark	:	Selbsteinstufung
Source	:	Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(9)

1.15 ADDITIONAL REMARKS

Remark : Possibilità di eliminazione

La sostanza ha una bassa solubilità in acqua (ca 0.1 mg/l); può essere eliminata per ossidazione biologica in appositi impianti di trattamento.
La sostanza può essere eliminata anche per ossidazione termica in appositi impianti di incenerimento con recupero energetico e controllo emissioni all'atmosfera secondo la normativa vigente.

Informazioni relative al trasporto

La sostanza che viene importata ed utilizzata come materia prima viaggia su carri cisterna ferroviari secondo la normativa Internazionale RID appartenendo alla classe 3 ordinale 32° c), indice KEMLER e n° ONU 30/1987.

Tipo del numero: ferrocisterna per prodotti RID

Quantità media
trasportata : 56.000 kg

Ferrocisterne/mese: 4

Misure di controllo
durante il trasporto: Il prodotto viaggia con la
documentazione stabilita dalle
leggi vigenti in materia
(normativa RID)

Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Remark : Wasserschadstoffklasse 2
Source : BUNA GMBH Schkopau

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value : -76 - 70 ° C
Source : Neste Oxo AB Stenungsund

(10)

Value : -76 - 70 ° C
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(11)

Value : -76 - 70 ° C
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(11)

Value : < -60 - ° C
Sublimation :
Method : other: DIN 3016
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund

(12)

Value : < -60 - ° C
Sublimation :
Method : other: DIN 3016
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main

(8)

Value : < -60 - ° C
Sublimation :
Method : other: DIN 3016
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

2.2 BOILING POINT

Value : = 184.5 - ° C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : = 184.5 - ° C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : = 184.5 - ° C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : = 184.5 - ° C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : = 184.5 - ° C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : = 184.5 - ° C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

2.3 DENSITY

Type : density
Value : = .83 - g/cm3 at 20° C
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(11)

Type :
Value : ca. .832 - .833 at 20° C
Source : ECEM European Chemical Marketing B.V. Amsterdam

Type : density
Value : = .832 - g/cm3 at 20° C
Method : other: DIN 51757
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund

(13)

Type : density
Value : = .832 - g/cm3 at 20° C
Method : other: DIN 51757
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main

(8)

Type : density
Value : = .832 - g/cm3 at 20° C

Method	:	other: DIN 51757
Year	:	
GLP	:	
Test substance	:	
Source	:	Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(9)

Type	:	density
Value	:	= .84 - g/cm3 at 20° C
Source	:	BASF AG Ludwigshafen

(14)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .05 - at 20° C
Source	:	ECEM European Chemical Marketing B.V. Amsterdam

Value	:	.144 - hPa at 20° C
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(15)

Value	:	= .144 - hPa at 20° C
Source	:	BASF AG Ludwigshafen

(15)

Value	:	.4 - hPa at 20° C
Decomposition	:	
Method		other (calculated): calculated
Year	:	
GLP	:	
Test substance	:	
Source	:	Neste Oxo AB Stenungsund

(13)

Value	:	= .4 - hPa at 20° C
Decomposition	:	
Method		other (calculated)
Year	:	
GLP	:	
Test substance	:	
Source	:	Hoechst AG Frankfurt/Main

(8)

Value	:	= .4 - hPa at 20° C
Decomposition	:	
Method		other (calculated)
Year	:	
GLP	:	

Test substance	:	
Source	:	Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(9)

Value	:	ca. .13 - hPa at 25° C
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(16)

Value	:	2.9 - hPa at 50° C
Decomposition	:	
Method		other (calculated): calculated
Year	:	
GLP	:	
Test substance	:	
Source	:	Neste Oxo AB Stenungsund

(13)

Value	:	= 2.9 - hPa at 50° C
Decomposition	:	
Method		other (calculated)
Year	:	
GLP	:	
Test substance	:	
Source	:	Hoechst AG Frankfurt/Main

(8)

Value	:	= 2.9 - hPa at 50° C
Decomposition	:	
Method		other (calculated)
Year	:	
GLP	:	
Test substance	:	
Source	:	Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(9)

2.5 PARTITION COEFFICIENT

Log pow	:	= 2.28 - at ° C
Method		other (calculated): calculated; Leo and Hansch
Year	:	
GLP	:	
Test substance	:	
Source	:	Neste Oxo AB Stenungsund

(13)

Log pow	:	= 2.28 - at ° C
Method		other (calculated): Leo und Hansch
Year	:	
GLP	:	
Test substance	:	
Source	:	Hoechst AG Frankfurt/Main

(8)

Log pow	:	= 2.28 - at ° C
Method		other (calculated): Leo und Hansch
Year	:	
GLP	:	
Test substance	:	
Source	:	Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(9)

Log pow	:	2.809 - at ° C
Method		other (calculated)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Calculated according to Leo and Hansch, MedChem-Programm, Version 1989 (POMONA89)
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

Log pow	:	ca. 3 - at ° C
Source	:	BASF AG Ludwigshafen

(17)

Log pow	:	= 3.1 - at ° C
Method		OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year	:	1981
GLP	:	no data
Test substance	:	
Source	:	Neste Oxo AB Stenungsund

(18)

Log pow	:	= 3.1 - at ° C
Method		OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year	:	1981
GLP	:	no data
Test substance	:	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(19)

Log pow	:	= 3.1 - at ° C
Method		OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year	:	1981
GLP	:	no data
Test substance	:	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(19)

2.6.1 WATER SOLUBILITY

Value : = .1 - at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Source : ECEM European Chemical Marketing B.V. Amsterdam

Value : ca. 1 - g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Source : Neste Oxo AB Stenungsund

(14)

Value : = 1 - g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : = 7 - at 1 g/l and 20 ° C
Source : Neste Oxo AB Stenungsund

(13)

Value : ca. 1 - g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Source : BASF AG Ludwigshafen

(15)

Value : = 1 - g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : = 7 - at 1 g/l and 20 ° C
Source : Hoechst AG Frankfurt/Main

(8)

Value : ca. 1 - g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(15)

Value : = 1 - g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : = 7 - at 1 g/l and 20 ° C
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : ca. 1 - g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : - at and ° C
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)

Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(15)

Value	:	= 1100 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(20)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 73 ° C
Type	:	closed cup
Source	:	ECEM European Chemical Marketing B.V. Amsterdam

Value	:	= 75 ° C
Type	:	
Method	:	other: DIN 51758
Year	:	
GLP	:	
Test substance	:	
Source	:	Neste Oxo AB Stenungsund

(13)

Value	:	= 75 ° C
Type	:	
Method	:	other: DIN EN 22719, ISO 2719
Year	:	
GLP	:	
Test substance	:	
Source	:	Hoechst AG Frankfurt/Main

(8)

Value	:	= 75 ° C
Type	:	
Method	:	other: DIN EN 22719, ISO 2719
Year	:	
GLP	:	
Test substance	:	
Source	:	Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(9)

Value	:	= 76 ° C
Type	:	
Method	:	other: DIN 51 758
Year	:	

GLP :
Test substance :
Source : Neste Oxo AB Stenungsund
BASF AG Ludwigshafen
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(15)

Value : = 82 ° C
Type : closed cup
Method : other
Year :
GLP :
Test substance :
Remark : Method: DIN 51758
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(21)

2.8 AUTO FLAMMABILITY

Value : = 270 - ° C at
Method : other: DIN 51 794
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund
BASF AG Ludwigshafen
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(15)

Value : = 305 - ° C at
Method : other: DIN 51794
Year :
GLP :
Test substance :
Remark : Auto-ignition temperature
Source : Neste Oxo AB Stenungsund

(13)

Value : = 305 - ° C at
Method : other: DIN 51794
Year :

GLP :
Test substance :
Remark : Zuendtemperatur
Source : Hoechst AG Frankfurt/Main

(8)

Value : = 305 - ° C at
Method : other: DIN 51794
Year :
GLP :
Test substance :
Remark : Zuendtemperatur
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : 330 - ° C at
Method : other
Year :
GLP :
Test substance :
Remark : Method: DIN 51794
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(19)

2.9 FLAMMABILITY

Result : other: when heated vapors may form explosive mixtures with air
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2.10 EXPLOSIVE PROPERTIES

Result : other
Remark : Explosionsgrenze: 1.1 - 12.7 Vol.-%
Source : Hoechst AG Frankfurt/Main

(8)

Result : other
Remark : Explosionsgrenze: 1.1 - 12.7 Vol.-%
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Result : other: Explosionsgrenzen 1.1 - 7.4 Vol.%

Source : BASF AG Ludwigshafen
(14)

Remark : Explosive limits in air: 1.1 -12.7 vol-%
Source : Neste Oxo AB Stenungsund
(13)

2.11 OXIDIZING PROPERTIES

Source : Neste Oxo AB Stenungsund

2.12 ADDITIONAL REMARKS

Remark : Remark 1: Viscosity
12 mm2/s at 20 degrees C
35 mm2/s at 0 degrees C
Remark 2: Henry's law constant: 2.65 E-5 atm x m3 x mole-1
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(22) (23)

Remark : Dynamic viscosity: 10 mPas at 20 degrees C.

(Method: DIN 51562)
Source : Neste Oxo AB Stenungsund
(13)

Remark : Viskositaet: 8.8 mPa.s (20 Grad C)
Source : BASF AG Ludwigshafen
(14)

Remark : Dynamische Viskositaet bei 20 Grad C: 10 mPas
(Methode: DIN 51562)
Source : Hoechst AG Frankfurt/Main
(8)

Remark : Dynamische Viskositaet bei 20 Grad C: 10 mPas
(Methode: DIN 51562)
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

Remark : Gefährliche Reaktionen: mit Oxidationsmitteln
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(9)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spect.	:	- nm
Rel. intensity	:	- based on Intensity of Sunlight
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	= .00000000001296 cm3/(molecule*sec)
Degradation	:	ca. 50 - % after 9.9 hour(s)
Deg. Product	:	
Method	:	other (calculated): calculated; AOPWIN, Version 1.55, April 1994, Syracuse Research
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	No study located.
Source	:	Neste Oxo AB Stenungsund

Type	:	air
Light source	:	
Light spect.	:	- nm
Rel. intensity	:	- based on Intensity of Sunlight
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	= .00000000001296 cm3/(molecule*sec)
Degradation	:	ca. 50 - % after 9.9 hour(s)
Deg. Product	:	
Method	:	other (calculated): AOPWIN, Version 1.55, April 1994, Syracuse Research
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Hoechst AG Frankfurt/Main Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(24)

3.1.2 STABILITY IN WATER

Remark	:	Study not located.
Source	:	Neste Oxo AB Stenungsund

3.1.3 STABILITY IN SOIL

Remark	:	Koc = 105 (calculated by equation 4-5 in Lyman, et al (1981).
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(25)

3.2 MONITORING DATA

Type of measurement : background concentration
Medium : surface water
Method :
Concentration : -
Result : 66-111 ug/l in Hayashida river, Japan.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(26)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration : -
Result : 3.0-5.0 ug/l in Delaware river (winter), USA, 1977.
Source : Neste Oxo AB Stenungsund

(27)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration : -
Remark : 2-Ethylhexanol detected in Mersey estaury 1990.
Source : Neste Oxo AB Stenungsund

(28)

Type of measurement : background concentration
Medium : drinking water
Method :
Concentration : -
Remark : 2-Ethylhexanol detected in "tap water", Japan 1980.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(29)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration : -
Result : 3.0-5.0 ug/l in Delaware river (winter), USA, 1977.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(27)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration : -
Remark : 2-Ethylhexanol detected in Mersey estaury 1990.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(28)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration : -
Result : 3.0-5.0 ug/l in Delaware river (winter), USA, 1977.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(27)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration : -
Remark : 2-Ethylhexanol detected in Mersey estaury 1990.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(28)

Type of measurement :
Medium : surface water
Method :
Concentration : -
Result : Saskatchewan River, 8 and 20 km downstream from Nipawin, 2-ethylhexanol detected, not quantified.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(30)

Type of measurement :
Medium : surface water
Method :
Concentration : -
Result : West Valley, New York: 3.6-8.1 mg/l
Source : Neste Oxo AB Stenungsund

(31)

Type of measurement :
Medium : surface water
Method :
Concentration : -
Result : West Valley, New York: 3.6-8.1 mg/l
Source : Neste Oxo AB Stenungsund

ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(31)

Type of measurement :
Medium : surface water
Method :
Concentration : -
Result : West Valley, New York: 3.6-8.1 mg/l
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(31)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Remark : No study located.
Source : Neste Oxo AB Stenungsund

3.3.2 DISTRIBUTION

Media : other
Method : Calculation according Mackay, Level I
Year :
Remark : Media: air-water-sediment-soil.

Result: air 16%, water 53%, sediment 25%, soil 5.4
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(32)

3.4 MODE OF DEGRADATION IN ACTUAL USE

Remark : Biological degradation is expected to be the main mode of degradation.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic, non-adapted

Concentration	:	3.16mg/l related to DOC (Dissolved Organic Carbon) related to
Contact time	:	
Degradation	:	= 55 - % after 17 day
Result	:	
Deg. Product	:	
Method	:	Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year	:	1984
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The test was performed on the sodium salt, which immediately dissociates to form the alcohol under the test conditions.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(33)

Type	:	aerobic
Inoculum	:	activated sludge, domestic, non-adapted
Concentration	:	6.32mg/l related to DOC (Dissolved Organic Carbon) related to
Contact time	:	
Degradation	:	= 68 - % after 17 day
Result	:	
Deg. Product	:	
Method	:	Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year	:	1984
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The test was performed on the sodium salt, which immediately dissociates to form the alcohol under the test conditions.
Source	:	Neste Oxo AB Stenungsund

Type	:	aerobic
Inoculum	:	activated sludge, domestic, non-adapted
Concentration	:	6.32mg/l related to DOC (Dissolved Organic Carbon) related to
Contact time	:	
Degradation	:	= 68 - % after 17 day
Result	:	
Deg. Product	:	
Method	:	Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year	:	1984
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The test was performed on the sodium salt, which immediately dissociates to form the alcohol under the test conditions.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(33)

Type	:	aerobic
Inoculum	:	activated sludge, domestic, non-adapted
Concentration	:	6.32mg/l related to DOC (Dissolved Organic Carbon) related to
Contact time	:	

Degradation	:	= 68 - % after 17 day
Result	:	
Deg. Product	:	
Method	:	Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year	:	1984
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The test was performed on the sodium salt, which immediately dissociates to form the alcohol under the test conditions.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(33)

Type	:	aerobic
Inoculum	:	activated sludge, domestic
Concentration	:	250mg/l related to related to
Contact time	:	
Degradation	:	= 100 - % after 5 day
Result	:	inherently biodegradable
Deg. Product	:	
Method	:	OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year	:	1985
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(34)

Type	:	aerobic
Inoculum	:	activated sludge, industrial, non-adapted
Contact time	:	
Degradation	:	> 95 - % after 5 day
Result	:	
Deg. Product	:	
Method	:	OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year	:	1980
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Non-biological elimination: 20-30%
Source	:	Neste Oxo AB Stenungsund

(35)

Type	:	aerobic
Inoculum	:	activated sludge, industrial, non-adapted
Contact time	:	
Degradation	:	> 95 - % after 5 day
Result	:	
Deg. Product	:	
Method	:	OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year	:	1980

GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Eliminierung durch nicht biol. Vorgänge 20 - 30 %
Source : Hoechst AG Frankfurt/Main

(36)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Contact time :
Degradation : > 95 - % after 5 day
Result :
Deg. Product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1980
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Eliminierung durch nicht biol. Vorgänge 20 - 30 %
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(36)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Concentration : 249mg/l related to Test substance
related to
Contact time :
Degradation : = 97 - % after 7 day
Result :
Kinetic of test substance : 1 day = 23 - %

2 day = 36 - %
5 day = 96 - %
7 day = 97 - %
- %

Deg. Product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Concentration : 249mg/l related to Test substance
related to
Contact time :
Degradation : = 97 - % after 7 day
Result :
Kinetic of test substance : 1 day = 23 - %

2 day = 36 - %
5 day = 96 - %
7 day = 97 - %
- %

Deg. Product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : Hoechst AG Frankfurt/Main

(37)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Concentration : 249mg/l related to Test substance
related to
Contact time :
Degradation : = 97 - % after 7 day
Result :
Kinetic of test substance : 1 day = 23 - %

2 day = 36 - %
5 day = 96 - %
7 day = 97 - %
- %

Deg. Product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(37)

Type : aerobic
Inoculum : activated sludge, domestic
Concentration : 83mg/l related to Test substance
related to
Contact time :
Degradation : = 88 - % after 17 day
Result :
Deg. Product :
Method : other: EEC Directive 79-831 Annex V Part C
Year : 1984
GLP :
Test substance :
Remark : Degradation is the measured BOD as percent of ThOD.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(38)

Type : aerobic
Inoculum : other: Belebtschlamm einer kommunalen Klaeranlage
Concentration : 83mg/l related to Test substance
related to
Contact time :
Degradation : = 88 - % after 17 day
Result :
Deg. Product :
Method : other: EEC Directive 79-831 Annex V Part C: Methods for the determination of ecotoxicity. Degradation - Biotic Degradation. Manometric Respirometry
Year : 1984
GLP :

Test substance :
Remark : Der Abbauwert ist der gemessene biochemische Sauerstoff-bedarf BSB als Prozentwert des theoretischen Sauerstoff-bedarfs (ThSB).
Source : BASF AG Ludwigshafen

(39)

Type : aerobic
Inoculum : activated sludge, non-adapted
Remark : Method: BOD5-20 fresh and sea water.

Results: Fresh water Sea water

BOD5=26%	BOD5=58%
BOD10=75%	BOD10=64%
BOD15=78%	BOD15=84%
BOD20=86%	BOD20=100%

Source : Neste Oxo AB Stenungsund

(40)

Type : aerobic
Inoculum : activated sludge, non-adapted
Remark : Method: BOD5-20 fresh and sea water.

Results: Fresh water Sea water

BOD5=26%	BOD5=58%
BOD10=75%	BOD10=64%
BOD15=78%	BOD15=84%
BOD20=86%	BOD20=100%

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(41)

Type : aerobic
Inoculum : activated sludge, non-adapted
Remark : Method: BOD5-20 fresh and sea water.

Results: Fresh water Sea water

BOD5=26%	BOD5=58%
BOD10=75%	BOD10=64%
BOD15=78%	BOD15=84%
BOD20=86%	BOD20=100%

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(41)

Type : aerobic
Inoculum : aerobic microorganisms
Concentration : .1mg/l related to
related to
Remark : Test medium: pure bacteria culture suspension isolated from activated sludge.

Results: Normal sewage (domestic waste water)
0% degraded after 24 h.
100% degraded after 5.6 days.

Adapted sewage (industrial effluent)
100% degraded after 24h.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(42)

Type : aerobic
Inoculum :
Source : Neste Oxo AB Stenungsund

(43)

Type : aerobic
Inoculum :
Result : Method: Secondary effluent from municipal and industrial waste water treatment plants was used as seed (25-55 ml/l).

Results:	Municipal	Industrial
BOD5/COD	0.70	0.60
BOD10/COD	0.81	0.77
BOD20/COD	0.87	0.86

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Type : aerobic
Inoculum :
Result : Method: Secondary effluent from municipal and industrial waste water treatment plants was used as seed (25-55 ml/l).

Results:	Municipal	Industrial
BOD5/COD	0.70	0.60
BOD10/COD	0.81	0.77
BOD20/COD	0.87	0.86

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF : ca. 27 -
Elimination :
Method : other: Calcualtion based on water solubility
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund

(44)

BCF	:	ca. 27 -
Elimination	:	
Method	:	other: Calcualtion based on water solubility
Year	:	
GLP	:	
Test substance	:	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(45)

BCF	:	ca. 27 -
Elimination	:	
Method	:	other: Calcualtion based on water solubility
Year	:	
GLP	:	
Test substance	:	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(45)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Cyprinus carpio (Fish, fresh water)
Exposure period	:	43 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
LC0	:	96 - 144
Method	:	other: diatary exposure
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	No effect on mortality
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(46)

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	27 - 29.5
Method	:	other: in Anlehnung an EPA-Guideline
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(47)

Type	:	static
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no data
NOEC	:	= 10 -
LC50	:	29.7 -
Method	:	other: keine Angaben
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(45)

Type	:	other
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	5 day
Unit	:	mg/l
Analytical monitoring	:	no data
LC50	:	= 24 -
Method	:	other: keine Angaben
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Test condition	:	Species: fry, 0.15 g Test condition: 15 degrees C, pH=7

(48)

Type	:	other
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no data
LC50	:	> 7.5 -
Method	:	other: keine Angaben
Year	:	
GLP	:	no data
Test substance	:	no data
Remark	:	Fry, 0.15 g
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Test condition	:	20 degrees C; pH = 7

(48)

Type	:	flow through
Species	:	Cyprinus carpio (Fish, fresh water)
Exposure period	:	43 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
LC0	:	96 - 144
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Method: diatary exposure. Result: No effect on mortality.
Source	:	Neste Oxo AB Stenungsund

(46)

Type	:	flow through
Species	:	Leuciscus idus melanotus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	= 14 -
LC50	:	= 17.1 -
LC100	:	= 21 -
Method	:	Directive 84/449/EEC, C.1 "Acute toxicity for fish"
Year	:	1984
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(49)

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
LC50	:	27 - 29.5
Method	:	other
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund

(47)

Type	:	static
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
NOEC	:	= 10 -
LC50	:	29.7 -
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund

(45)

Type	:	static
Species	:	Salmo gairdneri (Fish, estuary, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	32 - 37
Method	:	other: Range finding acute toxicity test.
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA)

Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(50)

Type	:	other
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	5 day
Unit	:	mg/l
Analytical monitoring	:	
LC50	:	= 24 -
Source	:	Neste Oxo AB Stenungsund
Test condition	:	Species: fry, 0.15 g

Test condition: 15 degrees C, pH=7

(51)

Type	:	other
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
LC50	:	> 7.5 -
Remark	:	Fry, 0.15 g
Source	:	Neste Oxo AB Stenungsund
Test condition	:	20 degrees C; pH = 7

(48)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC50	:	39 -
Method	:	Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year	:	1984
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(19)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC50	:	39 -
Method	:	Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year	:	1984
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA)

Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(19)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no data
EC50	:	= 44 -
Method	:	OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(45)

Type	:	
Species	:	Artemia salina (Crustacea)
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no data
EC50	:	= 19 -
Method	:	other: keine Angaben
Year	:	
GLP	:	no data
Test substance	:	no data
Remark	:	Species: seawater
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(41)

Type	:	
Species	:	Artemia salina (Crustacea)
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC50	:	= 19 -
Remark	:	Species: seawater
Source	:	Neste Oxo AB Stenungsund

(41)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC50	:	39 -
Method	:	Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year	:	1984
GLP	:	yes

Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund

(52)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC50	:	= 44 -
Method	:	OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund

(53)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC50	:	= 26 -
Method	:	other: Screening test
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(54)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Chlorella emersonii (Algae)
Endpoint	:	growth rate
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no data
NOEC	:	= 10 -
EC50	:	10 - 50
Method	:	other: keine Angaben
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Method: 22 degrees C, air was passed through the culture.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(48)

Species	:	Chlorella emersonii (Algae)
Endpoint	:	growth rate
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no data
NOEC	:	= 10 -
EC50	:	10 - 50
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Method: 22 degrees C, air was passed through the culture.
Source	:	Neste Oxo AB Stenungsund

(55)

Species	:	Scenedesmus subspicatus (Algae)
Endpoint	:	growth rate
Exposure period	:	72 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	= -
EC10	:	= 3.2 -
EC50	:	= 11.5 -
EC90	:	ca. 41.1 -
Method	:	Directive 87/302/EEC, part C, p. 89 "Algal inhibition test"
Year	:	1988
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(56)

Species	:	Scenedesmus subspicatus (Algae)
Endpoint	:	growth rate
Exposure period	:	72 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC10	:	= 1.3 -
EC50	:	= 13.3 -
EC90	:	= 138.5 -
Method	:	other: Algal growth inhibition test, UBA
Year	:	1984
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(57)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type	:	aquatic
Species	:	Pseudomonas putida (Bacteria)
Exposure period	:	18 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC10	:	= 540 -
Method	:	other: DIN 38412 Part 8
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(19)

Type	:	aquatic
Species	:	Pseudomonas putida (Bacteria)
Exposure period	:	18 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC10	:	= 540 -
Method	:	other: DIN 38412 Part 8
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(19)

Type	:	aquatic
Species	:	activated sludge, domestic
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
SG	:	ca. 300 -
Method	:	ETAD Fermentation tube method "Determination of damage to effluent bacteria by the Fermentation Tube Method"
Year	:	1980
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	SG = Schädlichkeitsgrenze
Source	:	Hoechst AG Frankfurt/Main Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(36)

Type	:	aquatic
Species	:	activated sludge, domestic
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
SG	:	ca. 300 -
Method	:	ETAD Fermentation tube method "Determination of damage to effluent bacteria by the Fermentation Tube Method"
Year	:	1980
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4

Remark	:	SG= Schädlichkeitgrenze
Source	:	Neste Oxo AB Stenungsund

(35)

Type	:	aquatic
Species	:	Pseudomonas putida (Bacteria)
Exposure period	:	18 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC10	:	= 540 -
Method	:	other: DIN 38412 Part 8
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund

(58)

4.5.1 CHRONIC TOXICITY TO FISH

Remark	:	Study not located.
Source	:	Neste Oxo AB Stenungsund

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Remark	:	Study not located.
Source	:	Neste Oxo AB Stenungsund

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

Remark	:	No study located.
Source	:	Neste Oxo AB Stenungsund

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

Remark	:	Study not located.
Source	:	Neste Oxo AB Stenungsund

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

Remark	:	No study located.
Source	:	Neste Oxo AB Stenungsund

4.7 BIOLOGICAL EFFECTS MONITORING

Remark	:	Study not located.
Source	:	Neste Oxo AB Stenungsund

4.8 BIOTRANSFORMATION AND KINETICS

Remark	:	Study not located.
Source	:	Neste Oxo AB Stenungsund

4.9 ADDITIONAL REMARKS

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 3730 - mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: 99.5%
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(59)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	1516 - 2774 mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	no data
Source	:	Neste Oxo AB Stenungsund

(60)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	3870 - 5520 mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: technical grade
Remark	:	2-Ethylhexanol (technical grade) was administered to a total of 70 female rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(61)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 3700 -
Method	:	
Year	:	
GLP	:	no
Test substance	:	no data
Remark	:	Range of values: 3.61-5.52 ml/kg (3.0-4.6 g/kg) 2-Ethylhexanol was given undiluted; no further details reported.
Source	:	Neste Oxo AB Stenungsund

(62)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 7000 - mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	no data
Remark	:	Result: 49 male albino rats (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 5, 6, 8, 10, 12, and 15 g/kg bw. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(63)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	1516 - 2774 mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	no data
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(64)

Type	:	LD50

Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 3700 -
Method	:	
Year	:	
GLP	:	no
Test substance	:	no data
Remark	:	Range of values: 3.61-5.52 ml/kg (3.0-4.6 g/kg) 2-Ethylhexanol was given undiluted; no further details reported.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(65)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	1516 - 2774 mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	no data
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(64)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 3700 -
Method	:	
Year	:	
GLP	:	no
Test substance	:	no data
Remark	:	Range of values: 3.61-5.52 ml/kg (3.0-4.6 g/kg) 2-Ethylhexanol was given undiluted; no further details reported.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(65)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 3768 - mg/kg bw

Method	:	
Year	:	
GLP	:	
Test substance	:	no data
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(66)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	3280 - 4460 mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: technical grade
Remark	:	Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 70 male mice.
Source	:	Neste Oxo AB Stenungsund

(67)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	2870 - 3610 mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: 2-EH technical grade
Remark	:	Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 50 femal mice.
Source	:	Neste Oxo AB Stenungsund

(68)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 3580 - mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Remark	:	Range of values: 2900-4420 mg/kg 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and adminisered to a total of 70 male mice. The LD50 was calculated 2 days after the test substance administration

(no further details reported).

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(61)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 2500 - mg/kg bw
Method :
Year :
GLP : no
Test substance :
Remark : Range of values: 2090-3010 mg/kg.
2-Ethylhexanol (technical grade, undiluted) was administered to a total of 70 female mice. The LD50 was calculated 1 day after the test substance administration (no further details reported).

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(61)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : 3280 - 4460 mg/kg bw
Method :
Year :
GLP : no
Test substance : other TS: technical grade
Remark : Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 70 male mice.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(61)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : 2870 - 3610 mg/kg bw

Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: 2-EH technical grade
Remark	:	Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 50 femal mice.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(61)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	3280 - 4460 mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: technical grade
Remark	:	Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 70 male mice.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(61)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	2870 - 3610 mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: 2-EH technical grade
Remark	:	Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 50 femal mice.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(61)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 1470 - mg/kg bw
Source	:	Neste Oxo AB Stenungsund

(69)

Type	:	LD50
Species	:	rabbit
Strain	:	

Sex :
Number of animals :
Vehicle :
Value : = 1180 - mg/kg bw
Method :
Year :
GLP : no
Test substance :
Remark : 2-Ethylhexanol (technical grade, undiluted) was administered to a total of 12 male rabbits. The LD50 was calcualted 1 day after the test substance administration (no further details reported).
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(61)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 1470 - mg/kg bw
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(65)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 1470 - mg/kg bw
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(65)

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 600 - mg/kg bw
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : Result: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as

paleness of the kidney.

Source : Neste Oxo AB Stenungsund

(70)

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : 1220 - 2820 mg/kg bw
Method :
Year :
GLP :
Test substance : other TS: 2-EH technical grade
Remark : 2-Ethylhexanol (technical grade) was administered to a total of 12 male guinea pigs. The LD50 was calculated 1 day after the test substance administration.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(61)

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 600 - mg/kg bw
Method :
Year :
GLP : no
Test substance :
Remark : 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.
Source : Neste Oxo AB Stenungsund

(71)

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 600 - mg/kg bw
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : Result: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as

paleness of the kidney.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(63)

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 600 - mg/kg bw
Method :
Year :
GLP : no
Test substance :
Remark : 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(63)

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 600 - mg/kg bw
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : Result: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(63)

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 600 - mg/kg bw
Method :
Year :
GLP : no
Test substance :
Remark : 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63,

0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(63)

5.1.2 ACUTE INHALATION TOXICITY

Type : other
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 4 hour(s)
Remark : Result: 2 groups of 6 Sprague-Dawley rats (3 male, 3 female) were exposed once to a vapor concentration of 0.89 mg/l and an aerosol/vapor concentration of 5.3 mg/l. Exposure was for 4 hrs, followed by a 7-day observation period. All animals exposed to to 5.3 mg/l died within 48 hrs of exposure, while animals of the other exposure group survived.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(72)

Type : other
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: 99.5%
Remark : Result: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of toxicity were reduced motilty, slight to moderate dyspnoea, and moderate irritation of the eyes, nose , pharynx and snout. The symptoms had subsided in rats 1 hour after exposure.
Source : Neste Oxo AB Stenungsund

(73)

Type : other
Species : rat
Strain :
Sex :

Number of animals	:	
Vehicle	:	
Exposure time	:	6 hour(s)
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: 99.5%
Remark	:	Result: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of toxicity were reduced motilty, slight to moderate dyspnoea, and moderate irritation of the eyes, nose , pharynx and snout. The symptoms had subsided in rats 1 hour after exposure.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(59)

Type	:	other
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Exposure time	:	6 hour(s)
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: 99.5%
Remark	:	Result: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of toxicity were reduced motilty, slight to moderate dyspnoea, and moderate irritation of the eyes, nose , pharynx and snout. The symptoms had subsided in rats 1 hour after exposure.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(59)

Type	:	other
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Exposure time	:	
Value	:	44 - ppm
Remark	:	Result: 44 ppm 2-ethylhexanol caused a 50% reduction in respiratory frequency in mice.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

Celanese GmbH Frankfurt am Main

(74)

Type	:	other
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Exposure time	:	6 hour(s)
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: purity 99.5%
Remark	:	A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.
Source	:	Neste Oxo AB Stenungsund

(75)

Type	:	other
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Exposure time	:	6 hour(s)
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: purity 99.5%
Remark	:	A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(59)

Type	:	other
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Exposure time	:	6 hour(s)
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: purity 99.5%
Remark	:	A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.

Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(59)

Type	:	other: Dampfinhalation
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Exposure time	:	
Method	:	other: interne Richtlinie der Hoechst AG
Year	:	1951
GLP	:	no
Test substance	:	other TS
Remark	:	2 ml Substanz in 7 Liter Luftraum verdampft rufen keine Letalität hervor.
Source	:	Hoechst AG Frankfurt/Main Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Test condition	:	Substanzreinheit > 98 %

(76)

Type	:	other: Vapor inhalation
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Exposure time	:	
Method	:	other: guidelines of Hoechst AG
Year	:	1951
GLP	:	no
Test substance	:	other TS
Remark	:	2 ml of 2-Ethylhexanol (vapour) in 7 l of air resulted in no lethal effects.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Test condition	:	2-Ethylhexanol concentration: > 98%

(76)

Type	:	other
Species	:	guinea pig
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Exposure time	:	6 hour(s)
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: purity 99.5%
Remark	:	A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol

under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.

Source : Neste Oxo AB Stenungsund

(75)

Type : other
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: purity 99.5%
Remark : A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(59)

Type : other
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: purity 99.5%
Remark : A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(59)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :

Value	:	> 3000 - mg/kg bw
Method	:	OECD Guide-line 402 "Acute dermal Toxicity"
Year	:	1981
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(77)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 1980 - mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Source	:	Neste Oxo AB Stenungsund

(78)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 2600 - mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	2-ethylhexanol did not produce any clinical signs of toxicity.
Source	:	Neste Oxo AB Stenungsund

(75)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 1980 - mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(64)

Type	:	LD50

Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 2600 - mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	2-ethylhexanol did not produce any clinical signs of toxicity.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(59)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 1980 - mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(64)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 2600 - mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	2-ethylhexanol did not produce any clinical signs of toxicity.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(59)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	

Vehicle	:	
Route of admin.	:	i.p.
Exposure time	:	
Value	:	= 937 - mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: 2-EH technical grade
Remark	:	Range of values: 860-1020 mg/kg. 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 male rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source	:	Neste Oxo AB Stenungsund

(79)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	i.p.
Exposure time	:	
Value	:	568 - 739 mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: 2-EH technical grade
Remark	:	Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 femal rats.The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(80)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	i.p.
Exposure time	:	
Value	:	= 650 - mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Remark	:	Rats promtly developed an irregular gait, dragging of hind legs, breathing became gasping, even on lower doses; rats were sound asleep in 10 min.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA)

Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(81)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	i.p.
Exposure time	:	
Value	:	= 937 - mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: 2-EH technical grade
Remark	:	Range of values: 860-1020 mg/kg. 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 male rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(80)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	i.p.
Exposure time	:	
Value	:	= 937 - mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: 2-EH technical grade
Remark	:	Range of values: 860-1020 mg/kg. 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 male rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(80)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	i.p.
Exposure time	:	

Value	:	845 - 939 mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: 2-EH technical grade
Remark	:	Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 70 male mice.The LD50 was calculated 1 day after the administration of the test substance administration (no further details reported).
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(80)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	i.p.
Exposure time	:	
Value	:	726 - 801 mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: 2-EH technical grade
Remark	:	Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 femal mice. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source	:	Neste Oxo AB Stenungsund

(82)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	i.p.
Exposure time	:	
Value	:	726 - 801 mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: 2-EH technical grade
Remark	:	Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 femal mice. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(80)

Type	:	LD50

Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	i.p.
Exposure time	:	
Value	:	726 - 801 mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS: 2-EH technical grade
Remark	:	Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 femal mice. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(80)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	s.c.
Exposure time	:	
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Remark	:	Range of values: 6.67-13.0 ml/kg (5.54-10.79 g/kg). 2-Ethylhexanol was given to female rats; no further details given.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(65)

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	irritating
EC classification	:	
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1981
GLP	:	no

Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Method :2-Ethylhexanol was applied under occlusion to the skin of 3 male rabbits for 4 hours. Result: An irritation index of 6.75/8 was determined. redness: x=3.33 edema : x=4.00
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(83)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	moderately irritating
EC classification	:	
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Remark	:	Method: Single dermal application, shaved dorsal skin, 24 hr occlusion. Result: moderate irritation (scale:slight-moderate-marked-severe) Not classifiable according to current EEC directives.
Source	:	Neste Oxo AB Stenungsund

(75)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	
EC classification	:	
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Remark	:	Irritation Index: 3/10. Not classifiable according to current EEC directives.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(64)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	highly irritating
EC classification	:	
Method	:	other: guidelines of Hoechst AG
Year	:	1978
GLP	:	no
Test substance	:	no data
Remark	:	0.5 ml of 2-Ethylhexanol was applied under occlusion on unabraded skin for 1,2,4 and 24 hours. Irritation effects seen after 7 days were not reversible.
Source	:	Neste Oxo AB Stenungsund

(84)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	irritating
EC classification	:	irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	BASF AG Ludwigshafen

(85)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	highly irritating
EC classification	:	
Method	:	other: interne Richtlinie der Hoechst AG
Year	:	1978
GLP	:	no
Test substance	:	no data
Remark	:	0.5 ml okklusiv auf die unverletzte Haut, Einwirkzeit 1, 2, 4 und 24 Stunden. nicht einstufbar, Reizerscheinungen nach 7 Tagen nicht reversibel.
Source	:	Hoechst AG Frankfurt/Main Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(86)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	moderately irritating
EC classification	:	

Method	:	
Year	:	
GLP	:	no
Test substance	:	
Remark	:	Method: Single dermal application, shaved dorsal skin, 24 hr occlusion. Result: moderate irritation (scale:slight-moderate-marked-severe) Not classifiable according to current EEC directives.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(59)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	highly irritating
EC classification	:	
Method	:	other: guidelines of Hoechst AG
Year	:	1978
GLP	:	no
Test substance	:	no data
Remark	:	0.5 ml of 2-Ethylhexanol was applied under occlusion on unabraded skin for 1,2,4 and 24 hours. Irritation effects seen after 7 days were not reversible.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(86)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	moderately irritating
EC classification	:	
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Remark	:	Method: Single dermal application, shaved dorsal skin, 24 hr occlusion. Result: moderate irritation (scale:slight-moderate-marked-severe) Not classifiable according to current EEC directives.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(59)

Species	:	rabbit
Concentration	:	
Exposure	:	

Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	highly irritating
EC classification	:	
Method	:	other: guidelines of Hoechst AG
Year	:	1978
GLP	:	no
Test substance	:	no data
Remark	:	0.5 ml of 2-Ethylhexanol was applied under occlusion on unabraded skin for 1,2,4 and 24 hours. Irritation effects seen after 7 days were not reversible.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(86)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	
EC classification	:	
Method	:	Draize Test
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	2-Ethylhexanol resulted in the following median scores (based on the scoring system by Draize): 19 (24 hrs), 20 (72 hrs), 0 (7 days). Not classifiable according to current EEC directives.
Source	:	Neste Oxo AB Stenungsund

(87)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	irritating
EC classification	:	
Method	:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	:	1981
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Irritation Index: 28.6/110 cornea: x=1.44 iris: x=0.89 conjunctiva: redness: x=2.56 chemosis:x=0.78
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(88)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	
EC classification	:	
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Remark	:	Instillation into the conjunctival sac of 20 ug caused moderately severe irritation of the cornea. Not classifiable according to current EEC directives.
Source	:	Neste Oxo AB Stenungsund

(89)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	
EC classification	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	no data
Remark	:	The test substance was reported to be irritating to rabbit eyes; no details reported.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(90)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	
EC classification	:	
Method	:	Draize Test
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	2-Ethylhexanol resulted in the following median scores (based on the scoring system by Draize): 19 (24 hrs), 20 (72

hrs), 0 (7 days).
Not classifiable according to current EEC directives.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(59)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result :
EC classification :
Method :
Year :
GLP : no
Test substance :
Remark : Instillation into the conjunctival sac of 20 ug caused moderately severe irritation of the cornea.
Not classifiable according to current EEC directives.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(64)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result :
EC classification :
Method : Draize Test
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : 2-Ethylhexanol resulted in the following median scores (based on the scoring system by Draize): 19 (24 hrs), 20 (72 hrs), 0 (7 days).
Not classifiable according to current EEC directives.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(59)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result :
EC classification :
Method :
Year :
GLP : no
Test substance :
Remark : Instillation into the conjunctival sac of 20 ug caused

moderately severe irritation of the cornea.
Not classifiable according to current EEC directives.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(64)

5.3 SENSITIZATION

Type	:	Patch-Test
Species	:	human
Number of animals	:	
Vehicle	:	
Result	:	not sensitizing
Classification	:	
Method	:	other: Maximization test
Year	:	
GLP	:	no
Test substance	:	no data
Remark	:	In an attempt to induce sensitization in 29 volunteers, subjects were given five 48-hr closed patch tests (during a 10-day period) with 4% in petrolatum. None of the subjects showed any positive reactions when challanged 10-14 days after the induction phase by final 48-hr closed patch test with the 4% petrolatum mixture.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(91)

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	inhalation
Exposure period	:	90 days
Frequency of treatment	:	6 hours/day, 5 days/week (total of 65 exposures)
Post obs. period	:	none
Doses	:	0, 15, 40 and 120 ppm
Control group	:	yes
NOAEL	:	>= 120 - ppm
Method	:	OECD Guide-line 413 "Subchronic Inhalation Toxicity: 90-day Study"
Year	:	1981
GLP	:	yes
Test substance	:	other TS: purity 99.9%
Remark	:	10 animals/sex/dose were used. The concentration of 120 ppm corresponds to the calculated saturated vapor concentration at 20?C. Body weights were determined weekly. Clinical signs and findings were recorded. Ophthalmologic examinations were carried out and blood was taken from all animals at the end

of the 3-month exposure period. Nummerous clinicochemical and hematological parameters, and various enzyme activites were measured and a clotting time analysis wes performed. The animals were sacrificed at the end of the 3-month exposure period and a complete necrpsy of all animals including weighing of certain organs and a gross-pathologic evaluation was performed; selected organs/tissues were examined histologically.

Result : Under the conditions of the test no treatment-related toxic effects were found in male and female Wistar rats which were exposed to 2-ethylhexanol vapor up to 120 ppm.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(92)

Species : rat
Sex : male/female
Strain : Wistar
Route of admin. : inhalation
Exposure period : 90 Tage
Frequency of treatment : 6 Std./Tag, 5 Tage/Woche
Post obs. period : keine
Doses : 0.081; 0.216; 0.648 mg/l (15; 40; 120 ppm) als Dampf
Control group : yes
NOAEL : .648 - mg/l
Method : OECD Guide-line 413 "Subchronic Inhalation Toxicity: 90-day Study"
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : Je 10 maennliche und 10 weibliche Tiere wurden in die Kontroll- und Versuchsgruppen eingesetzt.
Es wurden in keiner Versuchsgruppe substanzbedingte Veraenderungen festgestellt. Untersucht wurden klinische, ophthalmologische, haematologische und klinisch-chemische Parameter. Nach Versuchsende wurden die Tiere pathologisch untersucht.

Source : BASF AG Ludwigshafen

(93)

Species : rat
Sex : male/female
Strain : Wistar
Route of admin. : inhalation
Exposure period : 14 Tage
Frequency of treatment : 6 Std./Tag, 5 Tage/Woche
Post obs. period : keine
Doses : 0.16; 0.32, 0.65 mg/l (30; 60; 120 ppm) als Dampf
Control group : yes
NOAEL : .32 - mg/l
Method : other
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : Es handelte sich um eine Range-finding-study fuer einen

		90-Tageversuch. Keine substanzbedingten Veraenderungen wurden festgestellt, mit Ausnahme einer leichten Induktion der Cyanid-insensitiven Palmitoyl-CoA-Oxidase-Aktivitaet im Leberhomogenat der Tiere der hoechsten Dosisgruppe.
Source	:	BASF AG Ludwigshafen

(94)

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	11 days
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	0, 0.46%, 0.92%, 1.38%, 2.75% microencapsulated 2-ethylhexanol in the diet
Control group	:	yes
NOAEL	:	< .46 - %
LOAEL	:	= .46 - %
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity 99.8%
Remark	:	Control: placebo microcapsules (3%9 in the diet.
Result	:	Result: 2-Ethylhexanol was administered to groups of 10 male and 10 female rats per dose. The administration of 0.46, 0.92, 1.38 and 2.75 % (w/w) 2-ethylhexanol corresponded to a mean daily substance intake of about 500, 980, 1430, 2590 mg/kg bw 2-ethylhexanol in the male rat and of about 540, 1060, 1580, 2820 mg/kg body weight in the female rats. In all dose groups test substance related toxic effects were observed. Typical findings were: 0.46% group:increased relative stomach weights in the females; decreased cholesterol in both sexes; decreased triglycerides and alanine-aminotransferase in the males. 0.92% group: increased relative liver and stomach weights in the animals of both sexes; increase in the absolute stomach weights in the females; decreased triglycerides and alanine-aminotransferase and increased total protein in the males; minimal diffuse hypertrophy of the hepatocytes in one female; slight diffuse hypertrophy of the hepatocytes in all male and female rats. 1.38% group: increased relative liver and stomach weights in the animals of both sexes; increase in the absolute liver weights in both male and female animals; increase in the absolute stomach weights in the females; decreased cholesterol in both sexes; decreased triglycerides and alanine-aminotransferase in the males and decreased platelets in the females; increased total protein in the males; slight diffuse hypertrophy of the hepatocytes in most male and female rats; focal or multifocal acanthosis in the epithelium of the forestomach of one female rat. 2.75% group: increased relative liver and stomach weights in the animals of both sexes; increase in the absolute liver weights in the male and female animals; decreased cholesterol, triglycerides, glucose,

alanine-aminotranferase, reticulocytes, platelets and mean corpuscular volume in both sexes; focal or multifocal acanthosis in the epithelium of the forestomach in a few males and females.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(95)

Species : rat
Sex : male
Strain : Fischer 344
Route of admin. : oral feed
Exposure period : 3 weeks
Frequency of treatment : daily
Post obs. period : none
Doses : 2% in the diet
Control group : yes
Method :
Year :
GLP :
Test substance : no data
Result : Result: Administration of 2-ethylhexanol (purity not reported) to rats induced a marked PROLIFERATION of HEPATIC PEROXISOMES together with a significant INCREASE in HEPATIC CATALASE and CARNITINE ACTEYLTRANSFERASE activity. SERUM TRIGLYCERIDES were significantly DECREASED.
Source : Neste Oxo AB Stenungsund

(96)

Species : rat
Sex : male/female
Strain : other: Dow-Wistar
Route of admin. : oral feed
Exposure period : 3 months
Frequency of treatment : daily
Post obs. period : none
Doses : 0.01, 0.05, 0.25, 1.25 % in the diet
Control group : yes
NOAEL : = .05 - %
LOAEL : = .25 - %
Method :
Year :
GLP : no
Test substance :
Result : Result: 10 male and 10 female rats per dose group were treated with 2-ethylhexanol. No mortality, appetite depression, body weight gain, or kidney weight effect was found associated with dosing. Typical findings were:

1.25% group: increased liver weights (absolute and relative) in both males and females; cortical degeneration of the kidney in the males; focal liver congestion and/or swelling in female rats; increased incidence and distribution of transitory hepatic diffuse cloudy swelling and also diffuse

cloudy swelling of the proximal convoluted kidney tubules.

0.25% group:A trend of the diffuse cloudy swelling of the liver and the kidney was suggested histologically although to a proportionally smaller degree, and believed to be fortuitous.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(97)

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : oral feed
Exposure period : 11 Tage
Frequency of treatment : kontinuierlich
Post obs. period : keine
Doses : 1; 2; 3; 6 % in Mikrokapseln im Futter entspr. 0.46; 0.92; 1.38; 2.75 % 2-Ethylhexanol
Control group : yes, concurrent vehicle
NOAEL : < .46 - %
Method : other
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : 10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Kein Tier starb waehrend der Versuchsdauer. Die durchschnittliche taegliche Substanzaufnahme wurde fuer die weiblichen Tiere mit 500; 980; 1430 und 2590 mg/kg und fuer die maennlichen Tiere mit 540; 1060; 1580; 2820 mg/kg angegeben.
In der 6 % Dosisgruppe wurde eine verminderte Trinkwasser- und Futteraufnahme waehrend der Versuchsdauer beschrieben. Das Koerpergewicht der Tiere war reduziert.
Klinisch-chemische Untersuchungen erbrachten erniedrigte Werte von Cholesterol, Glucose und Alanin-Aminotransferase. Eine Abnahme von Reticulocyten, Thrombocyten und MCV wurde bei beiden Geschlechtern, von MCH bei weiblichen Tieren festgestellt. Ein Ansteigen des Gesamtproteingehaltes und der Erythrocyten wurde gemessen. Absolutes und relatives Lebergewicht waren erhoeht, wie auch das relative Magengewicht. Nur bei einem weiblichen Tier wurden makroskopisch fokale Laesionen im Vormagen festgestellt, mikroskopisch wurden bei mehreren Tieren Akanthose (fokal und multifokal) im Epithel des Vormagens beobachtet. Eine leichte diffuse Hypertrophie von Hepatocyten wurden bei allen Tieren dieser Dosisgruppe festgestellt.
Auch in der 3 % und 2 % Dosisgruppe wurden die klinischen, klinisch-chemischen und haematologischen Veraenderungen, wie auch die pathologischen Organveraenderungen der hoechsten Dosisgruppe festgestellt.
Auch in der 1 % Dosisgruppe wurde bei den maennlichen Tieren eine reduzierte Futteraufnahme beobachtet, auch waren die Veraenderungen bei den untersuchten klinisch-chemischen Parametern noch festzustellen. Bei den weiblichen Tieren war

		das relative Magengewicht erhoeht. Aufgrund der Befunde muss der NOAEL unterhalb der niedrigsten Dosierung liegen, d.h. < 0.46 % 2-Ethylhexanol.
Source	:	BASF AG Ludwigshafen

(98)

Species	:	rat
Sex	:	male
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	3 weeks
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	2% in the diet
Control group	:	yes
Method	:	
Year	:	
GLP	:	
Test substance	:	no data
Result	:	Result: Administration of 2-ethylhexanol (purity not reported) to rats induced a marked PROLIFERATION of HEPATIC PEROXISOMES together with a significant INCREASE in HEPATIC CATALASE and CARNITINE ACTEYLTRANSFERASE activity. SERUM TRIGLYCERIDES were significantly DECREASED.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(99)

Species	:	rat
Sex	:	male
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	3 weeks
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	2% in the diet
Control group	:	yes
Method	:	
Year	:	
GLP	:	
Test substance	:	no data
Result	:	Result: Administration of 2-ethylhexanol (purity not reported) to rats induced a marked PROLIFERATION of HEPATIC PEROXISOMES together with a significant INCREASE in HEPATIC CATALASE and CARNITINE ACTEYLTRANSFERASE activity. SERUM TRIGLYCERIDES were significantly DECREASED.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(99)

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	drinking water
Exposure period	:	9 days
Frequency of treatment	:	daily

Post obs. period	:	none
Doses	:	0, 308, 636 ppm
Control group	:	yes, concurrent vehicle
NOAEL	:	= 636 - ppm
Method	:	other: according to TSCA and EPA guidelines
Year	:	1983
GLP	:	yes
Test substance	:	other TS: purity >99.5%
Result	:	Result: Per dose, groups of 10 male and 10 female rats were exposed to 2-ethylhexanol. There were no treatment-related effects on clinical signs of toxicity, food consumption, body weight, serum chemistry, hematology, organ weights, gross pathology, or anatomic pathology.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(100)

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	21 days
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	100, 300, 950 mg/kg/day (vehicle:corn oil)
Control group	:	yes, concurrent vehicle
LOAEL	:	100 - mg/kg
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Result: Subchronic toxicity was elvaluated in groups of 5 female and 5 male rats. There were no mortalities. Clinical observations included reduced body weight gain in high dose females. Necropsy revealed elevated absolute and realtive liver weights in high dose males and females in the 2 highest dose groups; elevated realtive kidney weights in high dose females and males; increased serum triglyceride levels in high dose males; increased lauric acid 11-and 12-hydroxylase activities in high dose females and males; a dose related reduction in neutral lipids in the livers of treated animals; a dose related increase in cyanide-insensitive palmitoyl CoA oxidation in females and males; slightly increased hepatic peroxisomes in high dose females and males.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(101)

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	3 months
Frequency of treatment	:	daily (5 days /week)
Post obs. period	:	none
Doses	:	25, 125, 250, 500 mg/kg (in aqueous emulsion)
Control group	:	yes, concurrent vehicle
NOAEL	:	= 125 - mg/kg
LOAEL	:	= 250 - mg/kg
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity >99.8%
Remark	:	Vehicle: bidistilled water containing 5 ug/ml Cremophor EL. Concurrently to the main study a limited study with the same dosing regimen using 3 animals/sex/dose was performed; at the end of the treatment period all animals were sacrificed and samples of liver tissues and bone marrow were prepared for electron microscopy investigations; liver homogenates were prepared for clinicochemical examinations;
Result	:	Result: Limited study: The oral administration of 2-ethylhexanol over a period of 3 months led to an impairment of feed consumption and body weight gain in the male and female animals of the 500 mg/kg dose group. The cyanide-insensitive palmitoyl CoA-oxidation in the liver of male and female rats was strongly induced in the 500 mg/kg dose group and less pronounced in the 250 mg/kg dose group, probably due to a proliferation of peroxisomes. No substance-related findings were observed in the other dose groups. NOEL: 125 mg/kg bodyweight LOEL: 250 mg/kg bodyweight Main study: Per dose group 10 male and 10 female rats were treated. After the 3-month administration of 2-ethylhexanol toxic effects occurred in male and female rats of the 500 and 250 mg/kg dose groups. Typical findings were: 25 and 125 mg/kg groups: no substance-related findings 250 mg/kg group: increased relative liver weights in both sexes; increased relative stomach weights in females; decrease in alkaline phosphatase and glucose in males; decrease in alanine-aminotransferase in female rats. 500 mg/kg group: increased relative liver and stomach weights in both sexes; increased relative liver weights in the animals of both sexes; increased absolute stomach weights in female rats; decrease in alanine-aminotransferase, glucose and cholesterol in both sexes; decrease in alkaline phosphatase in males; single or multiple slightly elevated foci in the mucosa of the forestomach of male and female rats; focal or multifocal

acantosis in the mucosa of the forestomach of one male and five female animals.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(102)

Species : rat
Sex : male
Strain : Wistar
Route of admin. : gavage
Exposure period : 7 days
Frequency of treatment : daily
Post obs. period : none
Doses : 0, 1335 mg/kg/day in corn oil
Control group : yes, concurrent vehicle
Method :
Year :
GLP : no
Test substance : no data
Result : Result: The oral administration of 1335 mg/kg 2-ethylhexanol to a group of 6 male Wistar rats resulted in increased relative liver weights as compared to the control. In addition, significantly increased activity of cytochrome P-459s and biphenyl-4-hydroxylase of the liver were observed. Microsomal glucose-6-phosphatase activity was significantly decreased, while liver succinate dehydrogenase and aniline-4-hydroxylase activities were similar to the control. In the liver, electronmicroscopy studies showed and increase in the number of peroxisomes and dilatation of the smooth endoplasmic reticulum.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(103)

Species : rat
Sex : male
Strain : Sprague-Dawley
Route of admin. : gavage
Exposure period : 5 days
Frequency of treatment : daily
Post obs. period :
Doses : 352 mg/kg
Control group :
Result : Result: In this study an examination was made of the effect of 2-ethylhexanol on body weight, liver weights and on testicular and prostate weight. The seminiferous tubules were examined histologically. No indications were found of any changes.

Source	:	Neste Oxo AB Stenungsund (104)
Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	11 days (9 applications)
Frequency of treatment	:	5 days/week
Post obs. period	:	none
Doses	:	0, 100, 330, 1000, 1500 mg/kg (in aqueous emulsion)
Control group	:	yes, concurrent vehicle
NOAEL	:	= 100 - mg/kg
LOAEL	:	330 - mg/kg
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity >99.8%
Remark	:	vehicle: bidistilled water containing 5 ul/100 ml Cremophor EL.
Result	:	Result:Per dose 10 male and 10 female animals were treated. The 9-fold administration of 2-ethylhexanol to rats at doses of 1000 and 1500 mg/kg body weight led to clear toxic signs like impairment of food consumption and body weight gain as well as ataxia and/or lethargy. No substance-related effects were observed in the 100 mg/kg dose group. 1500 mg/kg dose group: decrease of cholesterol, glucose and reticulocytes in the animal of both sexes; increase of alanine aminotransferase in the males; increased relative stomach, liver , kidney and brain weights and decreased relative spleen weights in both sexes; increased relative adrenal weight in the male and lung weight in the female animals; foci in the forestomach of 4 male and 7 female animals; hyperkeratosis and focal or multifocal acanthosis in the mucuos membrane of the forestomac of all rats as well as epithelial degeneration, ulceration and subcutaneous inflammatory edema in some animals; slight hypertrophy of hepatocytes in the liver of 8 male and female rats each; focal hepatocellular necrosis in 2 male and 1 female rat; parenchymal involution of lympho-reticular tissue in the spleen in both sexes; decreased thymus size and lymphocyte depletion and necrosis in animals of both sexes. 1000 mg/kg dose group: decrease of cholesterol and reticulocytes in both sexes; increased relative stomach, liver and kidney weights and decreased spleen weights in both sexes; increased relative brain weight in the femal rats; foci in the forestomach of 2 males; hyperkeratosis and focal or multifocal acantosis in the mucous membrande of the forestomach of most male and female rats as well as epithelial degeneration, ulceration and subcutaneous inflammatory edema; parenchymal involution of lymphoreticular tissue in the spleen of 5 female rats, decreased thymus size in 2 male and 5 female rats; lymphocyte depletion and necrosis in the thymus of some female rats. 330 mg/kg dose group: increased relative kidney weights of the female rats;

inflammatory edema in the forestomach of 1 female and decreased thymus size in 2 male and 1 female rat.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(105)

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 9 days
Frequency of treatment : 5 days + 2 days without treatment + 4 days
Post obs. period : none
Doses : 0.1, 0.33, 1.0, 1.5 ml/kg/day (=83, 275, 834, 1250 mg/kg/day)
Control group : yes
NOAEL : 83 - mg/kg
Method : other: according to TSCA and EPA guidelines
Year : 1983
GLP : yes
Test substance : other TS: purity >99.5%
Result : Result: Per dose, groups of 10 male and 10 female F-344 rats were exposed by oral gavage to 2-ethylhexanol (undiluted). Treatment resulted in a spectrum of treatment-related, dose-dependent toxic effects in male and female rats.

No treatment-related effects were observed for any in-life, clinical pathology, gross necropsy, or histopathology observations at the 0.1 ml/kg/day level.

Effects associated with the administration of 2-ethylhexanol in males and/or females at one or more of the three highest dose levels were decreased food consumption and body weights, decreased total leukocytes and lymphocytes, increased liver weight, increased stomach weight (associated with hyperkeratosis, mucosal hyperplasia, edema, exocytosis and gastritis of the forestomach, but not glandular stomach), decreased spleen weight, thymic atrophy and lymphoid cell degeneratiion.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(100)

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 11 days (9 applications)
Frequency of treatment : 5 days/week

Post obs. period	:	none
Doses	:	0, 100, 330, 1000, 1500 mg/kg (in propylene glycol)
Control group	:	yes, concurrent vehicle
NOAEL	:	< 100 - mg/kg
LOAEL	:	= 100 - mg/kg
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity >99.8%
Remark	:	Vehicle: propylene glycol
Result	:	Per dose group, 10 male and 10 female rats were treated. 1500 mg/kg b.w. 2-ethylhexanol proved to be lethal for all female animals and 6 of the male animals. Doses of 1500, 1000, and 330 mg/kg bw resulted in clinically observable toxic effects like lethargy, ataxia, and/or reduced food consumption accompanied by reduced body weight gain. 1500 mg/kg group: Extremly reduced feed consumption and body weight in the surviving males; decrease of cholesterol, alanine-aminotransferase, leucocytes, lymphocytes, monocytes, hemoglobin, hematocrit, meancell volume, mean corpuscular hemoglobin and reticulocytes; increase in neutrophilic polymorpho-nuclear granulocytes; increase in relative stomach, liver and kidney weights and decrease in relative spleen and testes weights; foci in the forestomach. 1000 mg/kg dose group: Reduced feed consumption and body weight in the animals of both sexes; decrease of cholesterol, alanine-aminotransferase, leucocytes, lymphocytes, monocytes, hemoglobin, hematocrit, mean cell volume and reticulocytes and increaseof the neutrophilic polymorphonuclear granulocytes in both sexes; decrease of the mean corpuscular hemoglobin in the males; increased relative stomach, liver and kidney and decreased relative spleen weights in both sexes; increased testes weights in males; foci in the forestomach of all animals and ulcer in the forestomach of 2 males. 330 mg/kg group: Decrease of alanine-aminotransferase, hemoglobin, hematocrit, mean cell volume and reticulocytes and increase in the neutrophilic polymorphonuclear granulocytes in the females: increased relative stomach weight in both sexes, increased relative liver weight in the female and increased testes weights in the male animals; foci in the forestomach of all animals. 100 mg/kg group: Decreased of alanine-aminotransferase in the females; decreased relative liver weights in the male animals.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(106)

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	11 days (9 applications)
Frequency of treatment	:	5 days /week
Post obs. period	:	none
Doses	:	100, 330, 1000, 1500 mg/kg (in corn oil)
Control group	:	yes, concurrent vehicle
NOAEL	:	= 100 - mg/kg
LOAEL	:	= 330 - mg/kg
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity >99.8%
Result	:	Per dose 10 male and 10 female animals were treated. The 9-fold administration of 2-ethylhexanol to rats at doses of 1000 and 1500 mg/kg bw led to clear toxic signs like impairment of food consumption and body weight gain as well as ataxia and/or lethargy, piloerection, and genital region smeared with urine in both sexes. Some of these toxic signs were also found in some animals of the 330 mg/kg dose group. 1500 mg/kg dose group: One female rat died during the conduct of the study; decrease of cholesterol, glucose, alanine-aminotransferase, leukocytes, lymphocytes, monocytes and reticulocytes in both sexes; lowering of mean cell volume and mean corpuscular hemoglobin in the females; increase in total protein and triglycerides in both sexes; increased relative stomach, liver and kidney and decreased relative spleen weights in both sexes; increased relative testes weights; thickening of the wall of the forestomach and foci in the forestomach in some males and females. 1000 mg/kg dose group: One male rat died during the conduct of the study; decrease of cholesterol, glucose, leukocytes, lymphocytes and reticulocytes in both sexes; decrease of monocytes and increase of total protein in the males and decrease of themean cell volume in the females; increased relative stomach,liver and kidney and decreased relative spleen weights in both sexes; increased relative testes weights; thickening of the wall and foci in the forestomach in some animals. 330 mg/kg dose group: Increased relative testes weights; thickening of the wall and foci in the forestomach in some animals. 100 mg/kg dose group: No substance-related findings.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(107)

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	11 Tage
Frequency of treatment	:	einmal taeglich, 5 Tage/Woche
Post obs. period	:	keine
Doses	:	100; 330; 1000; 1500 mg/kg in Maisoel appliziert
Control group	:	yes, concurrent vehicle
NOAEL	:	100 - 330 mg/kg
LOAEL	:	330 - mg/kg
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Testsubstanz wurde in 5 ml/kg Maisoel appliziert. In der 1500 mg/kg Dosisgruppe starb ein weibliches Tier waehrend der Versuchsdauer, in der 1000 mg/kg Dosisgruppe ein maennliches Tier. In der hoechsten Dosisgruppe waren Futteraufnahme und Koerpergewichtsentwicklung reduziert. Ataxie, gestraeubtes Fell und bei einigen Tieren Lethargie und Speichelfluss wurden beobachtet. Bei 9 weiblichen Tieren und einem maennlichen Tier war in der Genitalregion das Fell mit Urin verklebt. Klinisch-chemische und haematologische Untersuchungen zeigten reduzierte Cholesterin-, Glucose- und Alanin-Aminotransferase-Werte. Gesamtproteingehalt und Triglyceride waren erhoeht. Leukocyten-, Lymphocyten-, Monocyten und Reticulocytenzahl war verringert, bei den weiblichen Tieren war auch das mittlere Blutkoerperchenvolumen und der Hb-Faerbkoeffizient verringert. Die absoluten Organgewichte von Leber und Milz waren bei beiden Geschlechtern reduziert, die von Niere und Hoden waren bei den maennlichen Tieren reduziert, vom Magen erhoeht. Relativ waren Magen-, Leber- und Nierengewicht bei beiden Geschlechtern erhoeht und Milzgewicht verringert. Das relative Hodengewicht war erhoeht. Histologisch wurde eine Verdickung der Vormagenwand, bei einigen Tieren mit Focibildung, beschrieben. In der 1000 mg/kg Dosisgruppe wurden im wesentlichen noch die gleichen Symptome wie in der 1500 mg/kg Dosisgruppe beobachtet. 330 mg/kg bewirkten Ataxie, gestraeubtes Fell und Urin auf dem Fell im Genitalbereich nur noch bei einigen Tieren. Es wurden keine klinisch-chemischen wie auch haematologischen Veraenderungen festgestellt. Das relative Hodengewicht war erhoeht. Die Veraenderungen im Vormagen wurden nur noch bei 3 Tieren festgestellt. Bei den Tieren, die 100 mg/kg erhielten wurden keine substanzbedingten Veraenderungen festgestellt.
Source	:	BASF AG Ludwigshafen

(108)

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	11 Tage

Frequency of treatment	:	einmal taeglich, 5 Tage/Woche
Post obs. period	:	keine
Doses	:	100; 330; 1000; 1500 mg/kg in Propylenglykol appliziert
Control group	:	yes, concurrent vehicle
NOAEL	:	< 100 - mg/kg
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Je 10 maennliche und 10 weibliche Tiere wurden in die Versuchs- und Kontrollgruppen eingesetzt. Die Substanz wurde in je 5 ml/kg Propylenglykol appliziert. In der 1500 mg/kg Dosisgruppe starben alle weiblichen und 6 maennliche Tiere. Die Futteraufnahme und die Koerpergewichtsentwicklung der ueberlebenden Tiere war signifikant reduziert, die Trinkwasseraufnahme erhoeht. Ataxie, Lethargie, gestraeubtes Fell, Bewusstseinsverlust, Hypothermie und bei einigen Tieren Speichelfluss und Urin auf dem Fell im Genitalbereich wurden als klinische Veraenderungen beschrieben. Bei den ueberlebenden Tieren waren im Blut Cholesterin, die Alanin-Aminotransferase, Leukocyten, Lymphocyten, Monocyten, Haemoglobin, Haematokrit, MCV und MCH reduziert, neutrophile polymorphkernige Granulocyten erhoeht. Die relativen Magen-, Leber- und Nierengewichte waren erhoeht, relative Hoden- und Milzgewichte verringert. Absolut waren Magen- und Lebergewichte erhoeht, Milz- und Nierengewichte reduziert. Bei allen ueberlebenden Tieren wurden Foci im Vormagen festgestellt. 2 Tiere der 1000 mg/kg Dosisgruppe starben. Klinische, klinisch-chemische und haematologische Veraenderungen entsprachen im wesentlichen denen, die bei den ueberlebenden Tieren der 1500 mg/kg Dosisgruppe beschrieben wurden. In der 330 mg/kg Dosisgruppe wurden bei je 3 maennlichen und 3 weiblichen Tieren noch klinische Veraenderungen in Form von Ataxie und Lethargie beschrieben. Auch waren die klinisch-chemischen und haematologischen Parameter noch veraendert. Absolute und relative Magen- und Hodengewichte waren erhoeht, wie auch die relativen Lebergewichte bei weiblichen Tieren. Bei allen Tieren wurde Focibildung im Vormagen beschrieben. In der 100 mg/kg Dosisgruppe waren bei den weiblichen Tieren die Alanin-Aminotransferase vermindert. Bei den maennlichen Tieren wurden verringerte relative Lebergewichte beschrieben. Keine weiteren substanzbedingten Veraenderungen wurden festgestellt. Der NOEAL liegt unter 100 mg/kg.
Source	:	BASF AG Ludwigshafen

(109)

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	11 Tage
Frequency of treatment	:	einmal taeglich, 5 Tage/Woche
Post obs. period	:	keine
Doses	:	100; 330; 1000; 1500 mg/kg in waessriger Emulsion appliziert
Control group	:	yes, concurrent vehicle

NOAEL	:	100 - 330 mg/kg
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Je 10 maennliche und 10 weibliche Tiere wurden in die Kontroll- und Versuchsgruppen eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser appliziert dem 5 ul/100 ml Cremophor EL zugesetzt waren. Kein Tier starb waehrend der Versuchsdauer. In der 1500 mg/kg Dosisgruppe war die Futteraufnahme und das Koerpergewicht der Tiere reduziert. Klinische Veraenderungen waren Ataxie, Lethargie, z.T. erschienen die Tiere bewusstlos, gestraeubtes Fell und Urin auf dem Fell im Genitalbereich. Die Cholesterol- und Glucosewerte waren reduziert, die Alanin-Aminotransferase bei den maennlichen Tieren erhoeht. Die Reticulocytenzahl war vermindert. Das absolute Organgewicht von Milz, Gehirn und Nebenniere war reduziert, das von Leber und Magen erhoeht. Relativ waren Magen-, Nieren-, Leber- und Gehirngewicht erhoeht, das relative Nebennierengewicht war bei den maennlichen Tieren und das relative Lungengewicht bei den weiblichen Tieren erhoeht. Das relative Milzgewicht war bei beiden Geschlechtern reduziert. Makroskopisch wurden im Vormagen bei den meisten Tieren Foci festgestellt. Histologisch wurden Hyperkeratosen, Akanthosen (fokal, multifokal) in der Vormagenschleimhaut bei allen Tieren beschrieben, bei einigen Tieren wurden epitheliale Degenerationen, Ulcerationen und subkutane entzuendliche Oedeme beschrieben. Bei einigen Tieren wurde eine leicht Hypertrophie der Hepatocyten, fokale hepatocellulaere Nekrosen und eine Rueckbildung des lymphoreticularen Gewebes festgestellt. Eine Verminderung der Thymusgroesse wurde bei fast allen Tieren beobachtet, wie auch eine Lymphocytendepletion im Thymus, bei einigen Tieren Lymphocytennekrosen. In der 1000 mg/kg Dosisgruppe wurden die gleichen Veraenderungen wie in der hoechsten Dosisgruppe beschrieben. In der 330 mg/kg Dosisgruppe waren die relativen Nierengewichte der weiblichen Tiere erhoeht. Die Thymusgroesse war bei 3 Tieren vermindert, bei einem weiblichen Tier wurden entzuendliche Oedeme im Vormagen festgestellt. Keine weiteren substanzbedingten Veraenderungen wurden beschrieben. 100 mg/kg bewirkte keine substanzbedingten Effekte.
Source	:	BASF AG Ludwigshafen

(110)

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	3 Monate
Frequency of treatment	:	einmal taeglich, 5 Tage/Woche
Post obs. period	:	keine
Doses	:	25; 125; 250; 500 mg/kg als waessrige Emulsion appliziert
Control group	:	yes, concurrent vehicle
NOAEL	:	125 - 250 mg/kg
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Result : Je 10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 10 ml/kg Wasser appliziert, dem 5 ul/100 ml Cremophor EL zugesetzt waren. Keine Tiere starben waehrend der Versuchsdauer.
In der hoechsten Dosisgruppe war sowohl die Koerpergewichtsentwicklung wie auch das Koerpergewicht der Tiere reduziert. Alanin-Aminotransferase, Glucose- und Cholesterolspiegel waren vermindert bei beiden Geschlechtern, bei den maennlichen Tieren war die alkalische Phosphatase vermindert, der Gesamtprotein- und Albumingehalt erhoeht. Ein Ansteigen der Reticulocyten wurde beschrieben. Absolute und relative Magen- und Lebergewichte waren erhoeht. Focibildung in der Schleimhaut des Vormagens wurde beschrieben. Histologisch wurden bei einigen Tieren Akanthose der Mucosa im Vormagen beschrieben. Bei einigen Tieren traten fettige Infiltrationen in der Leber (lobulaere Peripherie) auf.
In der 250 mg/kg Dosisgruppe wurden keine klinischen Veraenderungen festgestellt. Bei den maennlichen Tieren waren die alkalische Phosphatase und der Glucosespiegel reduziert, bei weiblichen Tieren die Alanin-Aminotransferase erhoeht. Das relative Lebergewicht war bei beiden Geschlechteren erhoeht, das relative Magengewicht nur bei weiblichen Tieren. Bei mikroskopischen Untersuchungen wurden geringgradige Fetteinlagerungen in den Leberzellen festgestellt.
In der 125 und 25 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt.

Es wurde zusaetzlich eine Satellitenstudie mit je 3 maennlichen und weiblichen Tieren pro Versuchs- und Kontrollgruppe durchgefuehrt. Bei diesen Tieren wurde nach Versuchsende das Leber- und Knochenmarkgewebe fuer elektronenmikroskopischen Untersuchungen praepariert. Sowohl in der 250 wie auch 500 mg/kg wurde bei beiden Geschlechtern dosisabhaengig eine Induktion der Cyanid-resistenten (peroxisomalen) Palmitoyl-CoA-Oxidase festgestellt.

Source : BASF AG Ludwigshafen

(111) (112)

Species : rat
Sex : male
Strain : Sprague-Dawley
Route of admin. : gavage
Exposure period : 5 days
Frequency of treatment : daily
Post obs. period :
Doses : 352 mg/kg
Control group :
Result : Result: In this study an examination was made of the effect of 2-ethylhexanol on body weight, liver weights and on testicular and prostate weight. The seminiferous tubules were examined histologically. No indications were found of any changes.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(113)

Species : rat

Sex	:	male
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	5 days
Frequency of treatment	:	daily
Post obs. period	:	
Doses	:	352 mg/kg
Control group	:	
Result	:	Result: In this study an examination was made of the effect of 2-ethylhexanol on body weight, liver weights and on testicular and prostate weight. The seminiferous tubules were examined histologically. No indications were found of any changes.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(113)

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	dermal
Exposure period	:	9 days
Frequency of treatment	:	5 days treatment, 2 days no treatment, 4 days treatment
Post obs. period	:	none
Doses	:	0, 0.5, 1.0 ml/kg/day (=0, 417, 834 mg/kg/day)
Control group	:	yes
Method	:	other: according to TSCA and EPA guidelines
Year	:	1983
GLP	:	yes
Test substance	:	other TS: purity >99.5%
Remark	:	Control: water
Result	:	Result: Per dose, groups of 10 male and 10 female F-344 rats were exposed to 2-ethylhexanol (undiluted, occluded cutaneous). Exposure was for 6 hours per treatment day. There were no treatment-related effects on clinical signs of toxicity, food consumption, or body weight following cutaeous exposure to 2-ethylhexanol. Lymphopenia and decreased spleen weight for high dose females and increased triglycerides for females at both dose levels compared to controls were observed. No other treatment-related effects on clinical pathology measurements or organ weights were observed for males or females at either dose level. Treatment-related anatomic and histologic lesions observed following cutaneous exposure to 2-ethylhexanol were restricted to the site of application and included exfoliation, acanthosis, hyperkeratosis, eschar formation, dermatitis and edema.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(100)

Species	:	rat

Sex	:	male
Strain	:	other
Route of admin.	:	dermal
Exposure period	:	16 days
Frequency of treatment	:	5 days/week
Post obs. period	:	14 days
Doses	:	0, 2.0 ml/kg/day
Control group	:	yes, concurrent no treatment
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Result	:	Result: 2.0 ml/kg/day 2-ethylhexanol (undiluted technical grade) was applied to the shaved back skin fo rats. Application was non occlusive, the animals were immobilized for two hours after the application. 5 animals were killed on the 17th day (the end of treatment period) and the remaining 5 on the 30th day (the end of observation period). On the 10th day a slight reddening and crusting of the skin was evident. The body weights on the 9th and 10th day, and the relative and absolute thymus weights on the 17th day, were significantly reduced. There were no effects on the weights of the heart, liver, spleen, or kidney, the level of protein, albumin, alpha-1-,beta-1-, and gamma-globulin content in serum. Histologically the following effects on organs were observed (with at least 3 out of 5 treated animals differing from the controls): Liver: histiocytic and inflammatory granulomas, peripheral fine-droplet fatty degeneration. Lungs: interstitial pneumonia, bronchiectasis, severe round-cell bronchitis. Kidneys: Epithelial-cell necrosis, cysts, basophilic "ballon nuclei". Heart: inter- and intracellular oedema, necrobiotic muscle fibres, interstitial oedema. Testes: interstitial oedema, reduced spermiogenesis. Thymus: increased "colliodocytes". Adrenals: Cortex very rich in lipoids. Histochemical investigation of the liver showed raised succinate-dehydrogenase activity and reduced lactate dehydrogenase activity. Tests on acid phosphatase and non-specific alpha-naphtylacetate esterase activity and on fat coloration gave no indications of any changes.
Source	:	Neste Oxo AB Stenungsund

(114)

Species	:	rat
Sex	:	male
Strain	:	other
Route of admin.	:	dermal
Exposure period	:	16 days
Frequency of treatment	:	5 days/week
Post obs. period	:	14 days
Doses	:	0, 2.0 ml/kg/day

Control group	:	yes, concurrent no treatment
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Result	:	Result: 2.0 ml/kg/day 2-ethylhexanol (undiluted technical grade) was applied to the shaved back skin fo rats. Application was non occlusive, the animals were immobilized for two hours after the application. 5 animals were killed on the 17th day (the end of treatment period) and the remaining 5 on the 30th day (the end of observation period). On the 10th day a slight reddening and crusting of the skin was evident. The body weights on the 9th and 10th day, and the relative and absolute thymus weights on the 17th day, were significantly reduced. There were no effects on the weights of the heart, liver, spleen, or kidney, the level of protein, albumin, alpha-1-,beta-1-, and gamma-globulin content in serum. Histologically the following effects on organs were observed (with at least 3 out of 5 treated animals differing from the controls): Liver: histiocytic and inflammatory granulomas, peripheral fine-droplet fatty degeneration. Lungs: interstitial pneumonia, bronchiectasis, severe round-cell bronchitis. Kidneys: Epithelial-cell necrosis, cysts, basophilic "ballon nuclei". Heart: inter- and intracellular oedema, necrobiotic muscle fibres, interstitial oedema. Testes: interstitial oedema, reduced spermiogenesis. Thymus: increased "colliodocytes". Adrenals: Cortex very rich in lipoids. Histochemical investigation of the liver showed raised succinate-dehydrogenase activity and reduced lactate dehydrogenase activity. Tests on acid phosphatase and non-specific alpha-naphtylacetate esterase activity and on fat coloration gave no indications of any changes.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(80)

Species	:	rat
Sex	:	male
Strain	:	other
Route of admin.	:	dermal
Exposure period	:	16 days
Frequency of treatment	:	5 days/week
Post obs. period	:	14 days
Doses	:	0, 2.0 ml/kg/day
Control group	:	yes, concurrent no treatment
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Result	:	Result: 2.0 ml/kg/day 2-ethylhexanol (undiluted technical

grade) was applied to the shaved back skin fo rats. Application was non occlusive, the animals were immobilized for two hours after the application. 5 animals were killed on the 17th day (the end of treatment period) and the remaining 5 on the 30th day (the end of observation period).

On the 10th day a slight reddening and crusting of the skin was evident. The body weights on the 9th and 10th day, and the relative and absolute thymus weights on the 17th day, were significantly reduced.

There were no effects on the weights of the heart, liver, spleen, or kidney, the level of protein, albumin, alpha-1-,beta-1-, and gamma-globulin content in serum.

Histologically the following effects on organs were observed (with at least 3 out of 5 treated animals differing from the controls):

Liver: histiocytic and inflammatory granulomas, peripheral fine-droplet fatty degeneration.
Lungs: interstitial pneumonia, bronchiectasis, severe round-cell bronchitis.
Kidneys: Epithelial-cell necrosis, cysts, basophilic "ballon nuclei".
Heart: inter- and intracellular oedema, necrobiotic muscle fibres, interstitial oedema.
Testes: interstitial oedema, reduced spermiogenesis.
Thymus: increased "colliodocytes".
Adrenals: Cortex very rich in lipoids.

Histochemical investigation of the liver showed raised succinate-dehydrogenase activity and reduced lactate dehydrogenase activity. Tests on acid phosphatase and non-specific alpha-naphtylacetate esterase activity and on fat coloration gave no indications of any changes.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(80)

Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	oral feed
Exposure period	:	11 days
Frequency of treatment	:	daily
Post obs. period	:	none
Doses	:	0.22, 0.44, 0.66, 1.32 % microencapsulated in the diet
Control group	:	yes, concurrent vehicle
NOAEL	:	= .44 - .66 %
LOAEL	:	= .66 - 1.32 %
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity >99.8%
Remark	:	NOEL: 0.44% = 1150 mg/kg/d (males) 0.66% = 2650 mg/kg/d (females) Control: placebo microcapsules (1.5%) in the diet.

Result	:	Result: 2-Ethylhexanol was administered to groups of 10 male and 10 female mice per dose. The administration of 0.22, 0.44, 0.66 and 1.32 % 2-ethylhexanol in the diet corresponded to a mean daily intake of about 550, 1150, 1800 and 4450 mg/kg b w 2-ethylhexanol for male mice and of about 750, 1750, 2650 and 5750 mg/kg bw for female mice. The only effect that could be assessed to be a substance related finding was the reduction in body weight gain in the male animals of the 0.66% group.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(115)

Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	oral feed
Exposure period	:	11 Tage
Frequency of treatment	:	kontinuierlich
Post obs. period	:	keine
Doses	:	0.48; 0.96; 1.44; 2.88 % in Mikrokapseln im Futter, entspr. 0.22; 0.44; 0.66; 1.32 % 2-Ethylhexanol
Control group	:	yes, concurrent vehicle
NOAEL	:	.44 - .66 %
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Es wurden je 10 maennliche und 10 weibliche Tiere in die Kontroll- und Versuchsgruppen eingesetzt. Die Substanzaufnahme wurde fuer die weiblichen Tiere mit 750; 1750; 2650 und 5750 mg/kg angegeben, fuer die maennlichen Tiere mit 550; 1150; 1800 und 4450 mg/kg. Kein Tier starb waehrend der Versuchsdauer. In der hoechsten Dosisgruppe wurde bei beiden Geschlechtern eine verminderte Koerpergewichtsentwicklung festgestellt, in der zweithoechsten Dosierung wurde dieses nur noch bei den maennlichen Tieren beobachtet. Es traten keine weiteren substanzbedingten Veraenderungen auf, untersucht wurden sowohl klinisch-chemisch und haematologisch Parameter, wie auch moegliche Organveraenderungen. Der NOEL wurde von den Autoren zwischen 0.44 und 0.66 % fuer maennliche Tiere und zwischen 0.66 und 1.32 % fuer weibliche Tiere angegeben. Der NOAEL liegt bei 1.32 % 2-Ethylhexanol.
Source	:	BASF AG Ludwigshafen

(116)

Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	gavage
Exposure period	:	11 days (9 applications)
Frequency of treatment	:	daily (9 applications)
Post obs. period	:	none

Doses	:	0, 100, 330, 1000, 1500 mg/kg (in corn oil)
Control group	:	yes, concurrent vehicle
NOAEL	:	= 330 - 1000 mg/kg bw
LOAEL	:	= 1000 - 1500 mg/kg bw
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity >99.8%
Remark	:	NOEL: 330 mg/kg (males) 1000 mg/kg (females)
Result	:	Result: 2-Ethylhexanol was administered to groups of 10 male and 10 female mice per dose. In the 1500 mg/kg dose group 1 male mouse died, 10 male and 5 female mice had clinical signs as ataxia, piloerection and lethargy. A few animals showed abdomnial position and loss of consciousness. An increase in the absolute and relative stomach weights was observed in male and female mice. In addition, male mice had decreased absolute and relative testes weights, and the relative liver and kidney weights of female mice were decreased.Gross lesions (foci in the mucosa) were seen in the forestomach of 7 male and 2 female mice. In the 1000 mg/kg dose group, a decrease in absolute and relative testes weights was observed. In the 100 and 330 mg/kg groups no substance-related findings were observed.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(117)

Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	gavage
Exposure period	:	3 months
Frequency of treatment	:	5 days per week
Post obs. period	:	none
Doses	:	25, 125, 250, 500 mg/kg (aqueous emulsion)
Control group	:	yes, concurrent vehicle
NOAEL	:	= 125 - 250 mg/kg
LOAEL	:	250 - 500 mg/kg
Method	:	
Year	:	
GLP	:	yes
Test substance	:	
Remark	:	Vehicle: bidistilled water containing 5 ug/100 ml Cremophore EL. Concurrently to the main study a limited study with the same dosing regimen using 3 animals/sex/dose was performed; at the end of the treatment period all animals were sacrificed for electron microscopic investigations; liver homogenates were prepared for clinicochemical examinations.
Result	:	Results:

Limited study: At the end of the 3-month administration period there were no substance-related clinical findings. There was no increase in the activity of the cyanide-insensitive palmitoyl-CoA-oxidation in the liver of the animals in all dose groups.

Main study: NOEL (females) = 250 mg/kg
NOEL (males) =125 mg/kg

2-Ethylhexanol was administered to groups of 10 male and 10 female mice per dose. After the 3-month administration of 2-ethylhexanol toxic effects affecting the stomach (increased weight and slight focal and multifocal acanthosis in the mucosa of the forestomach) occurred in the male and female animals of the 500 mg/kg dose group and in the male animals (increased relative weight) of the 250 mg/kg dose group. Clinically, none of the animals showed any abnormal signs which could be related to the test substance administration.No substance-related effects occurred regarding the clinical chemistry or hematology.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(118)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 11 days (9 applications)
Frequency of treatment : 5 days/week
Post obs. period : none
Doses : 0, 100, 330, 1000, 1500 mg/kg in propylene glycol
Control group : yes, concurrent vehicle
NOAEL : = 100 - mg/kg
LOAEL : = 330 - mg/kg
Method :
Year :
GLP : yes
Test substance : other TS: purity >99.8%
Result : Per dose group, 10 male and 10 female animals were treated. 1500 mg/kg and 1000 mg/kg 2-ethylhexanol being administered for 11 days (9 applications) proved to be a lethal dose for 4 male and 6 female (1500 mg/kg) or for 1 male and 1 female animal (1000 mg/kg), respectively. Doses of 1500 and 1000 mg/kg body weight resulted in clinically observable toxic effects like lethargy, ataxia, and/or reduced food consumption. Clinical chemistry and hematology did not show changes that could be related to the test substance administration.

1500 mg/kg dose group:
Increase relative stomach and liver weights in both sexes;increased relative spleen weight in female and decreased testes weights in the male mice; gross lesions

(foci of the mucosa, mainly white colored and slightly prominent) in the forestomach of the surviving animals of both sexes.

1000 mg/kg dose group:
Increased relative stomach and liver weights in both sexes; increased relative spleen weights in males; gross lesion (foci of the mucosa, mainly white colored and slightly prominent) in the forestomach of the surviving animals of both sexes.

330 mg/kg dose group:
Increased relative stomach and liver weights in the males; gross lesions (foci of the mucosa, mainly white colored and slightly prominent) in the forestomach of both sexes.

100 mg/kg dose group:
No substance-related findings

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(119)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 11 days (9 applications)
Frequency of treatment : 5 days/week
Post obs. period : none
Doses : 0, 100, 330, 1000, 1500 mg/kg (aqueous emulsion)
Control group : yes, concurrent vehicle
NOAEL : = 100 - mg/kg
LOAEL : = 330 - mg/kg
Method :
Year :
GLP : yes
Test substance : other TS: >99.8%
Remark : Vehicle: bidistilled water containing 5 ug/100ml Cremophor EL
Result : Per dose group, 10 male and 10 female animals were treated. The 9-fold application of 2-ethylhexanol led to substance induced clinical signs like ataxia and/or abnormal position in the male animals of the 330 mg/kg and 1500 mg/kg groups and in the female animals of the 1000 mg/kg and 1500 mg/kg groups. 1 male and 4 female mice of the 1500 mg/kg dose group and 1 female mouse of the 1000 mg/kg dose group died during the study. Clinical chemistry and hematology revealed no changes that could be attributed to the test substance.

1500 mg/kg dose group:
Increase in relative stomach and liver weights in both sexes; foci in the forestomach of males and females; hyperkeratosis and focal or multifocal acanthosis and inflammatory edema in the submucosa of the forestomach as well as focal or multifocal ulceration of the mucous

membrane in animals of both sexes; hypertophy of the hepatocytes in the liver in both sexes and focal necrosis of liver cells in one animal of both sexes: tubular giant cells in the testicular tubules in two male mice; tubular dilation and nephrosis in the renal cortex of animals that died intercurrently and centrilobular fatty infiltration in the liver of intercurrently died females.

1000 mg/kg dose group:
Increased relative liver weights in male and stomach weights in female mice; foci in the forestomach of some animals of both sexes; hyperkeratosis and focal or multifocal acanthosis and inflammatory edema in the submucosa of the forestomach as well as focal or multifocal ulceration of the mucous membrane in animals of both sexes; hypertrophy of hepatocytes in one male and one female animal; tubular dilation in the renal cortex and centrilobular fatty infiltration in the liver of the female mouse which died intercurrently.

330 mg/kg dose group:
Acanthosis in the mucous membrane of the forestomach of 2 male and 2 female mice, mostly connected with hyperkeratosis in the submucosa.

100 mg/kg dose group:
No substance-related findings.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(120)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 11 Tage
Frequency of treatment : einmal taeglich, 5 Tage/Woche
Post obs. period : keine
Doses : 100; 330; 1000; 1500 mg/kg in Maisoel appliziert
Control group : yes, concurrent vehicle
NOAEL : 330 - 1000 mg/kg
Method : other
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : 10 weibliche und 10 maennliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in je 5 ml/kg Maisoel appliziert.
In der 1500 mg/kg Dosisgruppe starb ein maennliches Tier waehrend der Versuchsdauer. Kein Effekt auf die Koerpergewichtsentwicklung wurde festgestellt. Bei allen maennlichen und 5 weiblichen Tieren dieser Dosisgrupppe wurde Ataxie, gestraeubtes Fell, Lethargie und bei einigen Tieren Bewusstlosigkeit beschrieben. Klinisch-chemische und haematologische Untersuchungen zeigten keine Veraenderungen.

Die absoluten Organgewichte vom Magen waren erhoeht, die der Hoden verringert. Auch die relativen Hodengewichte waren verringert, erhoeht waren die relativen Nieren- und Lebergewichte bei weiblichen Tieren und die relativen Magengewichte bei beiden Geschlechtern. Laesionen des Vormagens wurden bei 7 maennlichen und 2 weiblichen Tieren festgestellt.
In der 1000 mg/kg Dosisgruppe wurden bei den maennlichen Tieren verringerte absolute und relative Hodengewichte beschrieben, keine weiteren Veraenderungen wurden festgestellt.
In den beiden niederen Dosisgruppen wurden keine substanzbedingten Veraenderungen festgestellt.
Der NOAEL wurde fuer die maennlichen Tiere zwischen 330 und 1000 mg/kg angegeben, fuer die weiblichen Tiere zwischen 1000 und 1500 mg/kg.

Source : BASF AG Ludwigshafen

(121)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 11 Tage
Frequency of treatment : einmal taeglich, 5 Tage/Woche
Post obs. period : keine
Doses : 100; 330; 1000; 1500 mg/kg appliziert in Propylenglykol
Control group : yes, concurrent vehicle
NOAEL : 100 - 330 mg/kg
Method : other
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : Je 10 weibliche und 10 maennliche Tiere wurde pro Dosis- und Kontrollgruppe eingesetzt. Die Substanz wurde in 5 ml/kg Propylenglykol appliziert.
In der hoechsten Dosisgruppe starben 4 maennliche und 6 weibliche Tiere waehrend der Versuchsdauer. Bei den maennlichen Tiere wurde ein reduzierte Futteraufnahme, bei beiden Geschlechtern eine verminderte Wasseraufnahme festgestellt, die
Koerpergewichtsentwicklung war jedoch nicht signifikant beeinflusst. Klinische Veraenderungen waren Ataxie, Lethargie, bei einigen Tieren wurde gestraeubtes Fell, Dyspnoe, Hypothermie und Bewusstlosigkeit beschrieben. Keine Veraenderungen wurden bei klinisch-chemischen und haematologischen Untersuchungen festgestellt. Die absoluten Magen- und Lebergewichte waren erhoeht, die absoluten Hodengewichte verringert. Auch die relativen Magen- und Lebergewichte waren erhoeht, wie auch die relativen Milzgewichte bei den weiblichen Tieren. Bei den maennlichen Tieren waren die relativen Hodengewichte verringert. Bei den ueberlebenen Tieren dieser Dosisgruppe wurden Laesionen im Vormagen beschrieben.
2 Tiere der 1000 mg/kg Dosisgruppe starben waehrend der Versuchsdauer. Bei 6 maennlichen und 3 weiblichen Tieren der 1000 mg/kg Dosisgruppe wurden klinischen Veraenderungen festgestellt,
diese entsprachen denen in der hoechsten Dosisgruppe.
Veraenderte Organgewichte und Laesionen des Vormagens wurden auch in dieser Dosisgruppe festgestellt.

Bei den Tieren der 330 mg/kg Dosisgruppe wurden keine klinischen Veraenderungen festgestellt. Bei den Tieren wurden jedoch z.T. erhoehte Magen- und Lebergewichte festgestellt, auch zeigten die Tiere Laesionen im Vormagen.
In der 100 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt.

Source : BASF AG Ludwigshafen

(122)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 11 Tage
Frequency of treatment : einmal taeglich, 5 Tage / Woche
Post obs. period : keine
Doses : 100; 330; 1000; 1500 mg/kg in waessriger Emulsion appliziert
Control group : yes, concurrent vehicle
NOAEL : 100 - 330 mg/kg
Method : other
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : Je 10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser appliziert dem 5 ul/100 ml Cremophor EL zugesetzt wurden.
4 weibliche und 1 maennliches Tier der 1500 mg/kg Dosisgruppe, ein weibliches Tier der 1000 mg/kg Dosisgruppe und ein maennliches Tier der Kontrollgruppe starben waehrend der Versuchsdauer.
In der 1500 mg/kg Dosisgruppe wurde kein Effekt auf die Koerpergewichtsentwicklung festgestellt. Klinische Veraenderungen waren Ataxie, Lethargie, bei einigen Tieren gestraeubtes Fell und Bewusstlosigkeit. Klinisch-chemische und haematologische Untersuchungen zeigten keine Veraenderungen. Absolute und relative Leber- und Magengewichte waren erhoeht. Bei den meisten Tieren wurden Foci im Vormagen beschrieben. Histologisch wurde im Vormagen der Tiere Hyperkeratose, Akanthose (fokal, multifokal) und entzuendliche Oedeme der Submucosa beschrieben, bei einigen Tieren auch Ulcerationen der Schleimhaut. In der Leber wurde eine Hypertrophie der Hepatocyten, bei 2 Tieren fokale Nekrosen der Leberzellen beschrieben. Bei 2 maennlichen Tieren wurden tubulaere Riesenzellen bilateral in den testikulaeren Tubuli beobachtet. Tubulaere Dilatationen und Nephrosen der Nierenrinde wurden bei den Tieren, die waehrend des Versuchs starben festgestellt, bei einem Tier wurden auf centrilobulaer fettige Infiltrationen in der Leber festgestellt.
Auch in der 1000 mg/kg Dosisgruppe traten die Befunde der hoechsten Dosierung bei einigen Tieren auf.
In der 330 mg/kg Dosisgruppe wurden bei einem Tier klinische Veraenderungen (Ataxie, gestraeubtes Fell) beschrieben, auch wurden histologisch bei einigen Tieren im Vormagen Akanthose und Hyperkeratose der Schleimhaut festgestellt.
In der 100 mg/kg Dosisgruppe wurden keine substanzbedingten Effekte festgestellt.

Source : BASF AG Ludwigshafen

(123)

Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	gavage
Exposure period	:	3 Monate
Frequency of treatment	:	einmal taeglich, 5 Tage/Woche
Post obs. period	:	keine
Doses	:	25; 125; 250; 500 mg/kg
Control group	:	yes, concurrent vehicle
NOAEL	:	125 - 250 mg/kg
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Es wurden je 10 maennliche und 10 weibliche Tiere in die Versuchs- und Kontrollgruppen eingesetzt. Die Substanz wurde in 10 ml/kg Wasser appliziert, dem 5 ul/100 ml Cremophor EL zugesetzt waren. Ein Tier der 250 mg/kg Dosisgruppe starb waehrend der Versuchsdauer. In der 500 mg/kg Dosisgruppe wurden keine substanzbedingten klinischen, klinisch-chemischen und haematologischen Veraenderungen festgestellt. Das relative Magengewicht der maennlichen Tiere war erhoeht. Bei 2 maennlichen und einem weiblichen Tier wurde geringgradig Akanthose (fokal und multifokal) in der Mucosa des Vormagens beschrieben. In der 250 mg/kg Dosisgruppe wurde als einziger substanzbedingter Effekt ein erhoehtes relatives Magengewicht bei den maennlichen Tieren festgestellt. In der 25 und 125 mg/kg Dosisgruppe wurden keine Veraenderungen festgestellt. Es wurde zusaetzliche eine Satellitenstudie mit je 3 maennlichen und weiblichen Tieren pro Dosis- und Kontrollgruppe durchgefuehrt. Bei diesen Tieren wurde am Ende der Studie das Leber- und Knochenmarkgewebe fuer elektronenmikroskopische Untersuchungen praepariert. Es wurden keine substanzbedingten Effekte festgestellt. Keine Induktion der Cyanid-resistenten Palmitoyl-CoA-Oxidase wurde festgestellt.
Source	:	BASF AG Ludwigshafen

(124) (125)

Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration	:	up to 5000 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative

Method	:	other: according to Ames BN et al, Mutat Res 31, 347-364 (1975)
Year	:	1975
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(126)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537
Concentration	:	10, 33, 100, 220 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: according to Ames BN, et al. Mut Res 31, 347-364, 1975
Year	:	1975
GLP	:	no data
Test substance	:	other TS: Purity 99%
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(127)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration	:	0.01, 0.05, 0.25, 0.50, 1.0 ul/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: according to Ames BN, et al. Mut Res 31, 347-364, 1975.
Year	:	1975
GLP	:	yes
Test substance	:	no data
Remark	:	Solvent:DMSO
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(128)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration	:	0.002-1.8 ul/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: according to Ames BN,et al. Mut Res 31, 347-364 (1975)

Year	:	1975
GLP	:	yes
Test substance	:	no data
Remark	:	Solvent: DMF 2-Ethylhexanol was tested at dose levels of 0.002 to 1.8 ul/plate. In a separate toxicity test using the TA 100 strain, 80% toxicity was observed at 1.8 ug/plate in the absence of metabolic activation. The treatment did not induce statistically significant increases in the frequency of His+ revertants.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(129)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration	:	10, 100, 500, 1000, 5000 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	
GLP	:	yes
Test substance	:	no data
Remark	:	Solvent: ethanol. 2-Ethylhexanol was tested in the presence and absence of metabolic activation by Arochlor 1254-induced rat liver S9 fraction. Toxicity and precipitation were observed at the highest dose level in all tester strains. 2-Ethylhexanol did not induce a positive response in any tester strain with or wothout activation.
Source	:	Neste Oxo AB Stenungsund

(130)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration	:	4 to 2800 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS: purity >97%
Remark	:	2-Ethylhexanol was tested in the standard plate incorporation assay. Toxicity was observed in all tester strains at 2800 ug/plate.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(131)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538, TA 2637
Concentration	:	500 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	
GLP	:	
Test substance	:	
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(132)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration	:	1, 5, 10, 50, 100, 500, 1000 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: 2-EH 98%
Remark	:	Solvent: DMSO The preincubation method was used. Except for TA 1537 toxicity was observed at doses of 500 and 1000 ug/plate in all tester strains.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(133)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration	:	
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS: purity >97%
Remark	:	The mutagenicity of urin from Sprague-Dawley rats dosed daily by gavage for 15 days with 2,000 mg/kg of 2-ethylhexanol was evaluated. Cultures were dosed with up to 2 ml urine using direct plating procedures.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund

ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(134)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration	:	10, 100, 500, 1000, 5000 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	
GLP	:	yes
Test substance	:	no data
Remark	:	Solvent: ethanol. 2-Ethylhexanol was tested in the presence and absence of metabolic activation by Arochlor 1254-induced rat liver S9 fraction. Toxicity and precipitation were observed at the highest dose level in all tester strains. 2-Ethylhexanol did not induce a positive response in any tester strain with or wothout activation.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(135)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration	:	10, 100, 500, 1000, 5000 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	
GLP	:	yes
Test substance	:	no data
Remark	:	Solvent: ethanol. 2-Ethylhexanol was tested in the presence and absence of metabolic activation by Arochlor 1254-induced rat liver S9 fraction. Toxicity and precipitation were observed at the highest dose level in all tester strains. 2-Ethylhexanol did not induce a positive response in any tester strain with or wothout activation.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(135)

Type	:	Bacterial gene mutation assay
System of testing	:	Salmonella typhimurium TA 100
Concentration	:	0.5, 1.0, 1.5 mM
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	positive
Method	:	other: as described by author
Year	:	1982
GLP	:	no data

Test substance	:	no data
Remark	:	The mutagenic activity of 2-ethylhexanol was evaluated in an 8-azaguanine resistance assay. 2-ethylhexanolwas noted to be weakly mutagenic in a dose dependent way.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(136)

Type	:	Bacterial gene mutation assay
System of testing	:	Bacillus subtilis H17/M45
Concentration	:	500 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	
Result	:	negative
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(137)

Type	:	Cytogenetic assay
System of testing	:	Chinese hamster ovary (CHO) cells
Concentration	:	1.5-2.8 mM
Cycotoxic conc.	:	
Metabolic activation	:	
Result	:	ambiguous
Method	:	
Year	:	
GLP	:	
Test substance	:	
Remark	:	At 2.4 mM 2-ethylhexanol had a very slight effect on chromosomal integrity.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(138)

Type	:	DNA damage and repair assay
System of testing	:	E. coli strain W3110 (pol A+) and p3478 (pol A-)
Concentration	:	10, 50, 100, 250, 500 ug/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative

Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity 99.7%
Remark	:	2-Ethylhexanol was examined for DNA modifying activity in E. coli strain W3110 (pol A+) and its polymerase deficient derivative p3478 (pol A-). Based on a range finding study, the test article, dissolved in ethanol, was administered to cells at concentrations of 10, 50, 100, 250 and 500 ug/ml of bacterial suspension. Results were equivocal, however, as the test vehicle, ethanol, was found to be positive in the assay. The experiment was repeated using DMSO as the test vehicle and results were negative for 2-ethylhexanol.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(135)

Type	:	HGPRT assay
System of testing	:	CHO cells
Concentration	:	20-400 nl/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: as described by author
Year	:	1985
GLP	:	yes
Test substance	:	no data
Remark	:	2-Ethylhexanol was tested at concentrations of 20 to 300 nl/ml in the absence, and 100 to 400 nl/ml in the presence of Arochlor-induced rat liver S9 fraction. Reproducible increases in mutant frequencies of CHO-cells were not observed.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(139)

Type	:	Mouse lymphoma assay
System of testing	:	L5178Y TK+/- mouse lymphoma cells
Concentration	:	0.018, 0.024, 0.032, 0.042, 0.056, 0.075, 0.10, 0.13, 0.18,.0.24 ul/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: as described by author
Year	:	1983
GLP	:	yes
Test substance	:	other TS: purity >99.7%
Source	:	Neste Oxo AB Stenungsund

(140)

Type	:	Mouse lymphoma assay

System of testing	:	L5178Y TK+/- mouse lymphoma cells
Concentration	:	0.018, 0.024, 0.032, 0.042, 0.056, 0.075, 0.10, 0.13, 0.18,.0.24 ul/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: as described by author
Year	:	1983
GLP	:	yes
Test substance	:	other TS: purity >99.7%
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(128)

Type	:	Mouse lymphoma assay
System of testing	:	L5178Y TK+/- mouse lymphoma cells
Concentration	:	0.018, 0.024, 0.032, 0.042, 0.056, 0.075, 0.10, 0.13, 0.18,.0.24 ul/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: as described by author
Year	:	1983
GLP	:	yes
Test substance	:	other TS: purity >99.7%
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(128)

Type	:	Unscheduled DNA synthesis
System of testing	:	Primary rat hepatocytes
Concentration	:	2.5, 5, 10, 25, 50, 100, 250, 500 and 1000 nl/ml
Cycotoxic conc.	:	
Metabolic activation	:	without
Result	:	negative
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity > 99.7%
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(141)

Type	:	other: Cell transformation assay
System of testing	:	Balb/3T3 cells
Concentration	:	0.011 to 1.5.ul/ml
Cycotoxic conc.	:	
Metabolic activation	:	without
Result	:	negative
Method	:	other: as described by author
Year	:	1982
GLP	:	yes
Test substance	:	
Remark	:	2-Ethylhexanol was tested in the cell transformation assay in Balb/C-3T3 mouse embryo cells exposed to concentrations

of 1.5, 1.125, 0.75, 0.375, or 0.188 ul/ml under open vessel conditions, and 0.162, 0.129, 0.043 or 0.011 ul/ml under closed vessel conditions. No statistically significant increase in transformation rates was observed at any concentration.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(142)

Type : other: Cell transformation assay
System of testing : Balb/3T3 cells
Concentration : 0.011 to 1.5.ul/ml
Cycotoxic conc. :
Metabolic activation : without
Result : negative
Method : other: as described by author
Year : 1982
GLP : yes
Test substance :
Remark : 2-Ethylhexanol was tested in the cell transformation assay in Balb/C-3T3 mouse embryo cells exposed to concentrations of 1.5, 1.125, 0.75, 0.375, or 0.188 ul/ml under open vessel conditions, and 0.162, 0.129, 0.043 or 0.011 ul/ml under closed vessel conditions. No statistically significant increase in transformation rates was observed at any concentration.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(129)

Type : other: Cell transformation assay
System of testing : Mouse JB6 C141 cells
Concentration : 0.4 - 7.7 umol/l
Cycotoxic conc. :
Metabolic activation : without
Result : negative
Method : other: see reference
Year : 1986
GLP : no data
Test substance : no data
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(143)

Type : other: Cell transformation assay
System of testing : Balb/3T3 Clone A31 mouse embryo cells
Concentration : 30, 100 and 300 nl/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method :
Year :

GLP	:	yes
Test substance	:	other TS: purity > 99.7%
Source	:	Neste Oxo AB Stenungsund

(130)

Type	:	other: Cell transformation assay
System of testing	:	Balb/3T3 Clone A31 mouse embryo cells
Concentration	:	30, 100 and 300 nl/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity > 99.7%
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(135)

Type	:	other: Cell transformation assay
System of testing	:	Balb/3T3 Clone A31 mouse embryo cells
Concentration	:	30, 100 and 300 nl/ml
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity > 99.7%
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(135)

Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

5.6 GENETIC TOXICITY 'IN VITRO'

Type	:	Cytogenetic assay
Species	:	rat
Sex	:	male
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	5 days
Doses	:	0.02, 0.07, 0.21 ml/kg day
Result	:	
Method	:	other: as described by author
Year	:	1981
GLP	:	yes
Test substance	:	other TS: purity > 99.7%
Result	:	Result: Groups of 5 male F-344 rats were treated with

2-ethylhexanol. Of the 50 metaphase bone marrow cells examined from each animal, no significant increase in chromatid and chromosome breaks or structural rearrangements was noted. In addition, the mitotic index was unaffected by 2-ethylhexanol. At the dose levels tested 2-ethylhexanol did not induce detectable chromosomal aberrations after oral administration.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(144)

Type : Dominant lethal assay
Species : mouse
Sex : male
Strain : ICR
Route of admin. : oral unspecified
Exposure period : 5 days
Doses : 250, 500 and 1000 mg/kg
Result :
Method : other: as described by author
Year : 1981
GLP : yes
Test substance : other TS: purity 99.7%
Result : After treatment, each male was housed with 2 virgin females per week for 8 consecutive weeks to span the spermatogenic cycle. Females were sacrificed on day 14-17 of caging and scored for pregnancy, living fetuses and early and late fetal deaths. The fertility indicies and the average number of dead and total implants per pregnancy were within the normal range. It was concluded that 2-ethylhexanol did not induce dominant lethal mutations after oral administration.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(145)

Type : Drosophila SLRL test
Species : Drosophila melanogaster
Sex : male
Strain :
Route of admin. : other: injection
Exposure period : single application
Doses : 50000 ppm
Result :
Method : other: as described by author
Year : 1985
GLP : no data
Test substance : other TS: Purity>99%
Result : 2-Ethylhexanol was tested by injection in a solution of 0.7% aqueous NaCl. There was no mutagenic effect detectable.
Source : Neste Oxo AB Stenungsund

(146)

Type	:	Drosophila SLRL test
Species	:	Drosophila melanogaster
Sex	:	male
Strain	:	
Route of admin.	:	oral feed
Exposure period	:	72 hours
Doses	:	20000 ppm
Result	:	
Method	:	other: as described by author
Year	:	1985
GLP	:	no data
Test substance	:	other TS: 2-EH 99%
Result	:	Male flies were fed 2-ethylhexanol in a solution of 5% aqueous sucrose. The test substance was not mutagenic by this route.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(147)

Type	:	Drosophila SLRL test
Species	:	Drosophila melanogaster
Sex	:	male
Strain	:	
Route of admin.	:	other: injection
Exposure period	:	single application
Doses	:	50000 ppm
Result	:	
Method	:	other: as described by author
Year	:	1985
GLP	:	no data
Test substance	:	other TS: Purity>99%
Result	:	2-Ethylhexanol was tested by injection in a solution of 0.7% aqueous NaCl. There was no mutagenic effect detectable.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(147)

Type	:	Drosophila SLRL test
Species	:	Drosophila melanogaster
Sex	:	male
Strain	:	
Route of admin.	:	other: injection
Exposure period	:	single application
Doses	:	50000 ppm
Result	:	
Method	:	other: as described by author
Year	:	1985
GLP	:	no data
Test substance	:	other TS: Purity>99%
Result	:	2-Ethylhexanol was tested by injection in a solution of 0.7% aqueous NaCl. There was no mutagenic effect detectable.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA)

Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(147)

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	i.p.
Exposure period	:	single administration
Doses	:	456 mg/kg
Result	:	
Method	:	other: as described by author
Year	:	1982
GLP	:	yes
Test substance	:	no data
Result	:	B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 30 hrs post application and 1000 PCE/animal were scored for the presence of micronuclei. 2-Ethylhexanol was not considered to be clastogenic under the conditions of this assay.
Source	:	Neste Oxo AB Stenungsund

(148)

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	i.p.
Exposure period	:	single administration
Doses	:	456 mg/kg
Result	:	
Method	:	other: as described by author
Year	:	1982
GLP	:	yes
Test substance	:	no data
Result	:	B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 30 hrs post application and 1000 PCE/animal were scored for the presence of micronuclei. 2-Ethylhexanol was not considered to be clastogenic under the conditions of this assay.
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

(149)

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	i.p.
Exposure period	:	single administration
Doses	:	456 mg/kg
Result	:	
Method	:	other: as described by author
Year	:	1982
GLP	:	yes
Test substance	:	no data
Result	:	B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was

harvested 30 hrs post application and 1000 PCE/animal were scored for the presence of micronuclei. 2-Ethylhexanol was not considered to be clastogenic under the conditions of this assay.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(149)

Type : Micronucleus assay
Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : i.p.
Exposure period : two administrations
Doses : 456 mg/kg
Result :
Method :
Year :
GLP :
Test substance :
Result : B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 24 hrs after the second administation (the two administrations being 24 hrs apart) and 1000 PCE/animal were scored for the presence of micronuclei. 2-ethylhexanol was not considered to be clastogenic under the conditions of this assay.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(149)

5.7 CARCINOGENITY

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 24 months
Frequency of treatment : 5 days/week
Post. obs. period : none
Doses : 0, 50, 150, 500 mg/kg
Result :
Control group : yes, concurrent vehicle
Method : other: according to EPA-TSCA guidelines
Year :
GLP : yes
Test substance : other TS: purity 99.8%
Remark : Vehicle: aqueous 0.005% Cremophor EL.
In addition to the vehicle control groups, 50 rats/sex were dosed with water;
Concurrently to the main study, a satellite study was

performed. 2-Ethylhexanol was administered by gavage (same vehicle as in the main study) at a dose of 500 mg/kg. One group of rats (10/sex; interim sacrifice group) was treated with 2-ethylhexanol 5 days/week over a period of 18 months and then sacrificed. Another group (50 rats/sex; recovery group) was treated with the same dose for 18 months and thereafter with vehicle only for 6 months and then sacrificed. As a control group for the interim sacrifice group 10 male and 10 female rats received the vehicle for 18 months. Control data for the recovery group were adopted from the vehicle control group and the top dose group of the parallel main study.

Result : Result:

Satellite study:

In the interim sacrifice group a reduced body weight gain (both sexes) and clinical symptoms like poor general condition, labored breathing and "genital region smeared with urine" (females only) was observed. A slightly increased mortality in females was observed. The relative weight of testes and brain (males), stomach (females), liver and kidney (both sexes) were increased. In the recovery group similar effects were observed. After termination of treatment the body weight gain increased indicating a recovery effect. 18 males and 17 females died prematurely and one each had a focal hyperplasia in the forestomach. In the glandular stomach erosions were seen in 4 males and females each. Glandular cysts occurred in 6 males and 8 females.

Main study:

2-Ethylhexanol was not oncogenic in the rat under the conditions of this assay. In both sexes the sum of primary tumors, the sum of benign tumors and the sum of malignant tumors was lower in the top dose group than in either the vehicle control or the water control groups.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(150)

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 24 Monate
Frequency of treatment : einmal taeglich, 5 Tage/Woche
Post. obs. period : keine
Doses : 50; 150; 500 mg/kg
Result :
Control group : yes, concurrent vehicle
Method : other: EPA - TSCA oncogenicity guidelines, 798.3300
Year :
GLP : yes

Test substance : as prescribed by 1.1 - 1.4

Result : Es wurden je 50 maennliche und 50 weibliche Tiere in die Kontroll- und Versuchsgruppen eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser appliziert, dem 5 mg/100 ml Cremophor EL zugesetzt waren.
In der 50 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt.
150 mg/kg bewirkten eine Reduktion der Koerpergewichtsentwicklung bei den maennlichen Tieren um 16 % bei den weiblichen um 12 %. Es wurde eine leichte Zunahme der Anzahl von Tieren mit klinischen Veraenderungen (schlechter Allgemeinzustand, erschwerte Atmung, gestraeubtes Fell, Urin auf dem Fell im Genitalbereich) beschrieben.
Bei den Tieren der 500 mg/kg Dosisgruppe wurde eine starke Reduktion der Koerpergewichtsentwicklung festgestellt (31 - 33 %). Bei den weiblichen Tieren war die Mortalitaetsrate signifikant erhoeht (58 % gegenueber 28 % in der Kontrollgruppe). Die Zahl der Tiere mit klinischen Veraenderungen war erhoeht. Bei haemotologischen Untersuchungen wurde nach 12 Monaten Behandlungsdauer bei den maennlichen Tieren eine leichte Zunahme von Anisocytose, vorwiegend Microcytose, beschrieben. Dieser Befund wurde nach 18 und 24 Monaten nicht mehr festgestellt. Pathologisch wurde bei den Tieren eine Ansteigen der Bronchopneumonien beschrieben, das in Verbindung mit der Aspiration von Mageninhalten gesehen wurde. Es wurde keine erhoehte Tumorinzidenz festgestellt, die Summe der Tumoren war geringer als in der Kontrollgruppe.
Zur Hauptstudie wurde zusaetzlich eine Satellitenstudie mit der hoechsten Dosierung, 500 mg/kg durchgefuehrt. 2 Versuchsgruppen wurden eingesetzt, in der ersten Versuchsgruppe (10 maennliche und 10 weibliche Tiere) wurden die Tiere nach 18 Monaten getoetet und untersucht. In der 2 Versuchsgruppe (50 maennliche und 50 weibliche Tiere) wurden die Tiere 18 Monate mit der Substanz behandelt, danach 6 Monate entsprechend der Kontrolle.
Die Futteraufnahme war bei den maennlichen Tieren, die nach 18 Monaten getoetet wurden reduziert, die Koerpergewichtsentwicklung war bei den maennlichen Tieren um 28 % bei den weiblichen um 14 % reduziert. Eine Zunahme der Tiere mit schlechtem Allgemeinzustand wurde beschrieben, die Mortalitaet der weiblichen Tiere war erhoeht. Veraenderte Organgewichte wurden beschrieben.
Bei den Tieren, die nach 18 Monaten Behandlung eine 6-monatige Recovery-Phase hatte wurden folgende Veraenderungen beschrieben: reduzierte Futteraufnahme bei den maennlichen Tieren, die waehrend der Behandlung stark reduzierte Koerpergewichtsentwicklung war nach der Recovery-Phase weniger stark ausgepraegt. Klinischen Veraenderungen (schlechter Allgemeinzustand, erschwerte Atmung, Urin auf dem Fell in Genitalbereich) wurden festgestellt, auch die Organgewichte waren veraendert. Die Autoren sehen nur einen leichten Erholungseffekt waehrend der Recovery-Phase, aufgrund der Koerpergewichtsentwicklung.

Source : BASF AG Ludwigshafen

(151) (152)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage

Exposure period	:	18 months
Frequency of treatment	:	5 days/week
Post. obs. period	:	none
Doses	:	0, 50, 200, 750 mg/kg
Result	:	
Control group	:	yes, concurrent vehicle
Method	:	other: according to EPA-TSCA guidelines
Year	:	
GLP	:	yes
Test substance	:	other TS: purity 99.8%
Remark	:	Vehicle: aqueous 0.005% Cremophor EL In addition to the vehicle control groups, 50 mice/sex were dosed with water. Concurrently to the main study, a satellite study was performed: 2-Ethylhexanol was administered by gavage (same vehicle as in the main study) at a dose of 750 mg/kg. One group of mice (10/sex; interim sacrifice group) was treated with 2-ethylhexanol 5 days/week over a period of 13 months and then sacrificed. Another group (50 mice/sex; recovery group) was treated with the same dose for 13 months and thereafter with vehicle only for 5 months and then sacrificed. As a control group for the interim sacrifice group 10 male and 10 female mice received the vehicle for 13 months. Control data for the recovery group were adopted from the vehicle control group and the top dose group of the parallel main study.
Result	:	Result: Satellite study: The administration of 2-ethylhexanol to male and female mice for 13 months at a dose of 750 mg/kg caused increased mortality, reduced feed consumption and body weight gain in both sexes. The body weight gain of male and female animals of the recovery group were reduced as long as the animals were treated. After termination of treatment the male animals gained weight and reached nearly the values of the control group, indicating a recovery effect. No such effect was seen in females. Pathology revealed some statistically significant changes in organ weights and masses of foci in liver and stomach. One male and one female animal of the recovery group which died premarurely had a focal hyperplasia in the forestomach. Main study: 2-Ethylhexanol was not oncogenic in the mouse under the conditions of this assay. A slight increase in the incidence of hepatocellular carcinoma in the females of the high dose group was statistically significant if compared to the control group dosed with the emulsion vehicle, but not when compared to the control group dosed with water. This difference was regarded as incidental and not biologically relevant, based upon comparison with published data, and because of the lack of metastases. No statistically significant increase in tumor incidence occured in male mice.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA)

Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(153)

Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	gavage
Exposure period	:	18 Monate
Frequency of treatment	:	einmal taeglich, 5 Tage/Woche
Post. obs. period	:	keine
Doses	:	50; 200; 750 mg/kg
Result	:	
Control group	:	yes, concurrent vehicle
Method	:	other: EPA-TSCA oncogenicity guidelines (798.3300)
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Je 50 maennliche und 50 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser, dem 5 mg/100 ml Cremophor EL zugesetzt waren, appliziert. In der 50 und 200 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt. In der 750 mg/kg Dosisgruppe war die Koerpergewichtsentwicklung bei den maennlichen Tieren um 26 % bei den weiblichen um 24 % reduziert, verbunden mit einer reduzierten Futteraufnahme. Die Mortalitaet war signifikant erhoeht (30 % bei beiden Geschlechtern gegenueber 4 % bei maennlichen und 8 % bei weiblichen Kontrolltieren). Bei haematologischen Untersuchungen wurde ein leichter Anstieg der polymorphkernigen Neutrophilen und eine Verminderung der Leukocyten festgestellt. Im Vormagen der Tiere wurde eine Zunahme der fokalen Hyperplasien des Epithels beobachtet. Bei den weiblichen Tieren wurde ein leichter Anstieg der hepatocellulaeren Carcinome festgestellt, der im Vergleich zur Kontrolle signifikant war. Im Vergleich zu historischen Kontrollen war das vermehrte Auftreten von hepatocellaeren Carcinomen jedoch nicht signifikant, es wurden auch keine Metastasen festgestellt. Die Autoren beurteilen die Inzidenz der beobachteten Tumoren als zufaellig und ohne biologische Relevanz. Zur Hauptstudie wurde zusaetzliche eine Satellitenstudie durchgefuehrt. Die Tiere in der Satellitenstudie erhielten nur die hoechste Dosierung, d.h. 750 mg/kg. In der Satellitenstudie waren 3 Gruppen: eine Kontrollgruppe mit je 10 maennlichen und 10 weiblichen Tieren, eine Versuchsgruppe mit 10 weiblichen und 10 maennlichen Tieren, die Tiere dieser Gruppe wurden nach 13 Monaten Behandlung getoetet und eine weitere Versuchsgruppe mit je 50 maennlichen und 50 weiblichen Tieren, die 13 Monate behandelt wurden und danach bis zum Versuchsende (18 Monate) entsprechend der Kontrolle behandelt wurden. Veraenderungen bis zur Interimstoetung nach 13 Monaten waren: erhoehte Mortalitaet, reduzierte Futteraufnahme und reduzierte Koerpergewichtsentwicklung. In der Versuchsgruppe, in der die Tiere nach 13 Monaten

Substanzbehandlung noch 5 Monate beobachtete wurden, zeigten die maennlichen Tiere nach Absetzen der Behandlung eine deutliche Zunahme der Koerpergewichtsentwicklung, so dass nach 18 Monaten kein signifikanter Unterschied zu den Kontrollen festzustellen war. Bei den weiblichen Tieren wurde dieser Effekt nicht festgestellt.
Bei pathologischen Untersuchungen der behandelten Tiere wurden signifikante Unterschiede bei Organgewichten festgestellt, wie auch Focibildung in der Leber und im Magen.

Source : BASF AG Ludwigshafen

(154) (155)

5.8 TOXICITY TO REPRODUCTION

Remark : No study located.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : inhalation
Exposure period : gestation day 1 to 19
Frequency of treatment : daily (7 hours)
Duration of test : 20 days
Doses : 850 mg/m3
Control group : yes
Method : other: as described by author
Year : 1989
GLP : no data
Test substance : other TS: purity >99%
Result : Result: A group of Sprague-Dawley rats was exposed for 7 hours per day on gestation days 1-19 to 2-ethylhexanol at hte highest concentration that could be generated as a vapour. Dams were sacrificed on day 20. 2-Ethylhexanol reduced maternal feed intake, but did not produce any malformations.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(156)

Species : rat

Sex	:	female
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	gestation day 6 through 15
Frequency of treatment	:	daily
Duration of test	:	20 days
Doses	:	130, 650, 1300 mg/kg day (in bidist. water containing 0.005% Cremophor EL)
Control group	:	yes, concurrent vehicle
NOAEL Maternalt.	:	= 130 - mg/kg bw
NOAEL Teratogen	:	= 650 - 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: purity >99.5%
Result	:	Results:

2-Ethylhexanol was tested in this screening study (10 animals per dose group) for its prenatal toxicity in Wistar rats. On day 20 post coitum all surviving animals were sacrificed and assessed by gross pathology. The fetuses were dissected from the uterus, sexed, weighed and further investigated for any external, soft tissue and/or skeletal findings.

130 mg/kg dose group:
No adverse substance-related effects on dams of fetuses.

650 mg/kg dose group:
* maternal toxic effects
- 2 dams with piloerection
* embryo/fetotoxic effects
- slightly reduced mean fetal body weights
- increased frequency of fetuses with skeletal variations and retardations

1300 mg/kg dose group:
* maternal toxic effects
- markedly reduced food consumption during the whole treatment period (days 6-15 p.c.)
- distinctly reduced mean body weights (day 10 -20 p.c.) body weight loss during days 6-10 p.c. and reduced body body weight gains during days 10-15 p.c.; markedly reduced corrected body weight gain
- 6 animals found dead on days 9, 10 and 13 p.c.
- severe clinical sypmtoms like abdominal or lateral position, unsteady gait and apathy
- light brown-gray discoloration of the liver in the animals with intercurrent death; lund edema and emphysema in a few animals, and hemometra in 1 dam which showed vaginal hemorrage before death
- distinctly reduced mean uterus weight
* embryo/fetotoxic effects
- increased number of resorptions and consequently markedly increased postimplantation loss
- markedly reduced mean fetal body weights
- one fetus with acaudia and atresia ani; increased incidence of fetuses with dilated renal pelvis and/or hydroureter higher number of fetuses with skeletal malformations, variations and retardations.

Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(157)

Species	:	rat
Sex	:	female
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	single application on day 12 of gestation
Frequency of treatment	:	single application on day 12 of gestation
Duration of test	:	
Doses	:	6.25, 12.5 mmol/kg (833, 1666 mg/kg)
Control group	:	yes, concurrent no treatment
Method	:	other: as described by author
Year	:	1985
GLP	:	no data
Test substance	:	no data
Result	:	Results: The group given 833 mg/kg showed a slight increase of 2% in malformed fetuses relative to the controls (0%). The other parameters (implantation index, mean fetal weight, number of dead and resorbed fetuses) were unaffected. Simultaneous intraperitoneal administration of 150 mg caffeine / kg potentiated this effect (increase in malformed fetuses to 21.2 %). Even after a dose of 1666 mg/kg, the implantation index and percentage of dead and resorbed fetuses were unchanged, although the mean fetal body weight at 3.5 g was reduced relative to the controls (4.1 g). 22.2 % of the surviving fetuses showed malformations (controls 0%). These included hydronephrosis (7.8%), tail anomalies (4.9%), anomalies of the extremities (9.7%) and "others" (1%).
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(158)

Species	:	rat
Sex	:	female
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	6.- 15. Tag der Traechtigkeit
Frequency of treatment	:	einmal taeglich
Duration of test	:	bis zum 20. Tag der Traechtigkeit
Doses	:	130; 650; 1300 mg/kg
Control group	:	yes
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Result : Je 10 Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 5 ml/kg bidest. Wasser appliziert, das zu 0.005 % Cremophor EL enthielt.

Die niedrigste Dosierung hatte keine Wirkung auf die Muttertiere und Feten.

650 mg/kg fuehrten bei 2 Muttertieren zu gestraeubtem Fell. Das Fetengewicht war leicht reduziert und die Zahl der skelettalen Variationen und Retardierungen erhoeht.

1300 mg/kg bewirkten deutliche maternale Toxizitaet. 6 Muttertiere starben waehrend der Versuchsdauer. Die maternale Futteraufnahme war waehrend der Behandlungsdauer deutlich reduziert. Sowohl die Koerpergewichtsentwicklung wie auch das Koerpergewicht zu Versuchsende waren reduziert. Deutliche klinische Symptome traten auf. Bei den Tieren die waehrend der Behandlungsdauer starben wurden braun-graue Verfaerbungen der Leber beschrieben, Lungenoedeme und -emphyseme. Das Uterusgewicht war deutlich reduziert. Die Zahl der Resorptionen und Postimplantationsverluste war deutlich erhoeht, die Fetengewichte reduziert. Bei einem Fetus wurde Schwanzlosigkeit und Analatresie festgestellt. Die Zahl der Feten mit erweiterten Nierenbecken und Hydroureter war erhoeht, wie auch die Zahl der Feten mit skelettalen Missbildungen, Variationen und Retardierungen.

Source : BASF AG Ludwigshafen

(159)

Species : mouse
Sex : female
Strain : CD-1
Route of admin. : gavage
Exposure period : gestation day 7 through 14
Frequency of treatment : daily
Duration of test :
Doses : 1525 mg/kg
Control group : yes, concurrent vehicle
Method : Chernoff-Kavlok teratogenicity screening test
Year : 1980
GLP : yes
Test substance : no data
Remark : Vehicle : corn oil.

Observation period: until day 3 post partum.

The results of this study regarding the influence of 2-ethylhexanol on reproduction should be taken with care since the dose applied resulted in the death of more than 30 % of treated dams. Therefore, the observed effects on the offspring should be attributed to the extensive maternal toxicity and are very unlikely to be primary effects. The authors state that the results of this assay should not be used to label a chemical as teratogenic or nonteratogenic but to establish priorities for conventional testing.

Result : This screening test was conducted with one group of 50 pregnant CD-1 mice. The dose of 1525 mg 2-ethylhexanol/kg/day was determined previously as the minimal effective dose for adult female mice. In 17 animals, test substance related mortality was observed by the end of the treatment period. Another animal died because of a

dosing error. Clinical observations in dams included languidity, ataxia, coldness to touch, wet stains, oily coat, and dark red discharge from the anus of one animal. Decreases in body weights and the reproductive index were observed in treated animals compared to controls. Decreases were also observed in the following parameters when compared to controls: mean number of live pups per litter, litter weight, pup weight on days 1 and 3, percent change in pup weight from day 1 to day 3, mean pup viability per litter from day 1 to 3, and percent of live pups per litter on day 1 post partum. The mean number and percent of dead pups in the treatment group was reported to be greater than in the control group.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(160)

Species : mouse
Sex : female
Strain : CD-1
Route of admin. : oral feed
Exposure period : gestation day 0 through 17
Frequency of treatment : daily (microencapsulated in the diet)
Duration of test :
Doses : 0, 17, 59, 191 mg/kg/day
Control group : yes
NOAEL Maternalt. : > 191 - mg/kg bw
NOAEL Teratogen : > 191 - mg/kg bw
Method : other: as described by author
Year : 1991
GLP : yes
Test substance : other TS: purity >99%
Result : Result: No dams died, delivered early or were removed from the study. Pregnancy rate was high and equivalent across all groups. There was no treatment-related maternal toxicity observed in this study.

There were no effects of exposure to diatary 2-ethylhexanol on any gestational parameters. The number of corpora lutea, uterine implantation sites, pre- and postimplantation loss, sex ratio and live fetal body weight per litter were all equivalent across all groups. There were also no treatment-related changes in the incidence of individual, external, visceral, skeletal or total malformations or variations. In conclusion, there were no maternal or developmental toxic effects of 2-ethylhexanol dietary exposure throughout gestation at any concentration tested.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(161)

Species	:	rat
Sex	:	female
Strain	:	Fischer 344
Route of admin.	:	dermal
Exposure period	:	gestation day 6 through 15
Frequency of treatment	:	daily (6 hours)
Duration of test	:	21 days
Doses	:	0.3, 1.0, 3.0 ml/kg/day (252, 840, 2520 mg/kg/day)
Control group	:	yes
NOAEL Maternalt.	:	= 252 - 840 mg/kg bw
NOAEL Teratogen	:	> 2520 - mg/kg bw
Method	:	other: according to US EPA Health Effect Guidelines
Year	:	1989
GLP	:	yes
Test substance	:	other TS: purity >99.7%
Result	:	Result: Administration of 2-ethylhexanol by occluded cutaneous application to time-pregnant Fischer 344 rats during organogenesis at 0, 0.3, 1.0, or 3.0 ml/kg/day (25 animals per dose) resulted in maternal toxicity at 1.0 and 3.0 ml/kg/day (clinical signs of toxicity at the dosing site for both doses and reduced weight gain in the treatment period at 3.0 ml/kg/day), and no developmental toxicity at any doses tested. There was no treatment-related increased incidence of malformations at any dosage employed.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(162)

5.10 OTHER RELEVANT INFORMATION

Type	:	adsorption
Remark	:	The percutaneous absorption rate of [14C]-2-ethylhexanol through human stratum corneum and full thickness rat skin has been measured in vitro using Franz-type glass diffusion cells. The absorption rate of 2-ethylhexanol through rat skin was 190 +-40 and 240 +-110 ug/cm2/hr in two separate studies. Similarly, the absorption rate through human stratum corneum was found to be 39 +-16 and 37 +- 10 ug/cm2/hr in two separate studies. The overall mean rate of percutaneous absorption through rat skin is 5.7 times the rate through human stratum corneum.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

(163)

Type : adsorption
Remark : In vitro percutaneous absorption studies were carried out for eight chemicals, including 2-ethylhexanol, using full thickness rat skin and human stratum corneum. The purpose of the studies was to compare the rates of absorption for the two species. For each of the chemicals, the observed rate using full thickness rat skin was greater than that observed for human stratum corneum.
Source : Neste Oxo AB Stenungsund

(164)

Type : adsorption
Remark : In vitro percutaneous absorption studies were carried out for eight chemicals, including 2-ethylhexanol, using full thickness rat skin and human stratum corneum. The purpose of the studies was to compare the rates of absorption for the two species. For each of the chemicals, the observed rate using full thickness rat skin was greater than that observed for human stratum corneum.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(164)

Type : adsorption
Remark : In vitro percutaneous absorption studies were carried out for eight chemicals, including 2-ethylhexanol, using full thickness rat skin and human stratum corneum. The purpose of the studies was to compare the rates of absorption for the two species. For each of the chemicals, the observed rate using full thickness rat skin was greater than that observed for human stratum corneum.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(164)

Type : Biochemical or cellular interactions
Remark : The incubation of 325.6 to 1953.5 ug/ml 2-ethylhexanol with the 9000xg supernatant of rat liver homogenate dose dependently reduced the activities of the aniline hydroxylase and the aminopyrin-N-demethylase.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(165)

Type : Biochemical or cellular interactions
Remark : B6C3F1 mice received a diet with 1 % di(2-ethylhexyl)-adipate for 4 weeks, followed by single gavage administration of 110 or 120 mg 14C-2-ethylhexanol per kg body weight. In the liver DNA, only trace amounts of radioactivity could be detected, which were deduced to be caused by the incorporation of metabolites of ethylhexanol. A similar result was obtained with rats. These were pretrerated for 4 weeks with 1% di(2-ethylhexyl)-

phthalate in the diet and then received a single dose of 51 or 53 mg 14C-2-ethylhexanol /kg body weight.

Source : Neste Oxo AB Stenungsund

(166)

Type : Biochemical or cellular interactions
Remark : The ability of 2-ethylhexanol to promote the development of putative preneoplastic lesions was evaluated. GGT+ foci were initiated in the livers of male Sprague-Dawely rats with a single dose of diethylnitrosamine following partial hepatectomy. Rats were fed a 2-ethylhexanol (0.17%) containing diet for 10 weeks. The test material produced essentially no effect with regard to number of GGT+ foci, peroxisome proliferation or liver weight.
Source : Neste Oxo AB Stenungsund

(167)

Type : Biochemical or cellular interactions
Remark : The effect of 2-ethylhexanol on the dissociation of germinal cells from Sertoli cells in cultures of seminiferous tubule cell preparations was investigated. In contrast to mono-ethylhexyl-phthalate, a concentration of 26.1 ug/ml 2-ethylhexanol did not have a detectable effect on the germinal cell dissociation (incubation time was 48 hrs).
Source : Neste Oxo AB Stenungsund

(168)

Type : Biochemical or cellular interactions
Remark : Rats were fed ad libitum a diet containing 2% of 2-ethylhexanol for two weeks. At the end of this period the livers were removed, pieces were taken for electron microscopy, and the reminder was homogenized and subfractioned to obtain mitochondria and microsomes. Protein and various enzyme activities were measured. 2-Ethylhexanol did not have a detectable influence on peroxisomal palmitoyl -CoA oxidation, catalase, or urate oxidase, on mitochondrial protein content, cytochrome c oxidase, carnitine-acetyl transferase, or on microsomal protein content, cytochrome P-450 and NADPH-cytochrome c reductase.
Source : Neste Oxo AB Stenungsund

(169)

Type : Biochemical or cellular interactions
Remark : Adult rat hepatocytes cultured for 48 h in the presence of 1 mM 2-ethylhexanol contained increased numbers of peroxisomes. The peroxisome proliferation was associated with a marked increase (9-fold) in the activity of carnitine acetyltransferase.
Source : Neste Oxo AB Stenungsund

(170)

Type : Biochemical or cellular interactions
Remark : Primary rat hepatocyte cultures were used to compare the effects of some alkylphthalate esters on peroxisomal enzyme activities and morphology. Carnitine acteyltransferase activity in hepatocytes, treated with 1 mM (=130.2 ug/ml) 2-ethylhexanol for 48 hrs, was elevated 6-fold as compared to the control.
Source : Neste Oxo AB Stenungsund

(171)

Type : Biochemical or cellular interactions

Remark : 2-Ethylhexanol was fed to male Swiss-Webster mice at a concentration of 2 % in the diet for 10 days. Treatment resulted in increased absolute liver weights, increased cytosolic and microsomal epoxide hydrolase and GSH S-transferase activities, and an increased cytosolic and microsomal protein content of the liver, as compared to controls.

Source : Neste Oxo AB Stenungsund

(172)

Type : Biochemical or cellular interactions

Remark : Kupffer cells, the resident hepatic macrophages, are activated by calcium and release a variety of mitogenic growth factors that may modulate cell proliferation. In this study, the cytosolic free calcium concentration in Fura-2-loaded cultured Kupffer cells was increased significantly following incubation with Wy-14,643 (1.25 mM), while equimolar concentrations of 2-ethylhexanol had no effect. However, at higher concentraitons (3 nM), ethylhexanol also increased intracellular calcium.

Source : Neste Oxo AB Stenungsund

(173)

Type : Biochemical or cellular interactions

Remark : The dose response relationship for peroxisome proliferation due to 2-ethylhexanol was investigated in male and female Alderley Park rats (Wistar-derived and Fischer 344) and mice (Swiss and B6C3F1). The animals were administered 2-ethylhexanol for 14 consecutive days at doses from 0 to 1.05 g/kg/day for rats and 0 to 1.75 g/kg/day for mice. At doses above 1.05 g/kg/day, 2-ethylhexanol was toxic to male and female rats, leading to death of the animals. Relative liver weights were increased in a dose-related manner in both species and sexes examined. Essentially linear dose-response relationships were observed for the induction of peroxisomal beta-oxidation (measured as palmitoyl CoA oxidation activities) in rats and mice.

Source : Neste Oxo AB Stenungsund

(174)

Type : Biochemical or cellular interactions

Remark : Toxicity of 2-ethylhexanol was assessed in the perfused rat liver. Livers from starved rats were perfused with 2-ethylhexanol (3 mM) dissolved in O2/CO2-saturated buffer. Following infusion of ethylhexanol, O2 uptake and ketone body formation were diminished by 50 and 80%, respectilely, and cell damage, as assessed by the appearance of lactate dehydrogenase in the effluent perfusate, was apparent. Only O2-rich upstream regions of the liver lobule were damaged as reflected by trypan blue uptake. It is concluded, that the toxicity of ethylhexanol in the liver is dependent on local O2 tension and mitochondria are primary targets.

Source : Neste Oxo AB Stenungsund

(175)

Type : Biochemical or cellular interactions

Remark : 2-Ethylhexanol (70uM) stimulated oxygen uptake in the perfused rat liver by about 10 % during the first 10 min of infusion. Perfusions with a hepatotoxic dose of ethylhexanol (3 mM) led to a transient increase in oxygen uptake followed by a rapid inhibition of respiration of over 50 % in 10 min. Lactate dehydrogenase release, indicative of irreversible

cell death, was detected in the effluent perfusate after 20 min. Within 10 min of perfusion, ethylhexanol decreased the ATP/ADP ratio from 2.5 to 0.9. Thus, marked decreases in hepatic energy state due to inhibition of respiration pereceded cell death. The effect of ethylhexanol on isolated mitochondria was also studied: ethylhexanol stimulated state-4 rates of respiration, diminished coupled rates of respiration, and decreased the P/O ratio in a dose-dependent manner. It also decreased the uptake of radiolabelled CaCl2 by isolated mitochondria 4- to 5-fold. It was hypothesized, that ethylhexanol initially uncouples oxidative phosphorylation leading to diminished ATP synthesis and collapse of ion gradients across the mitochondrial membrane.

Source : Neste Oxo AB Stenungsund

(176)

Type : Biochemical or cellular interactions

Remark : 2-Ethylhexanol causes toxicity exclusively to periportal regions of the perfused liver. To determine whether this toxicity was due to local oxygen tension or to drug delivery, isolated cylinders (plugs) of periportal and pericentral regions of the liver lobule from rats pretreated with phenobarbital were collected. Incubation of plugs with 2-ethylhexanol (0.1 to 4 mM) diminished urea synthesis in a dose-related manner and caused extensive cell damage. Plugs isolated from both regions of the liver lobule were affected similarly by ethylhexanol and O2. The data indicate, that ethylhexanol toxicity is dependent on oxygen tension in isolated sublobular regions of the liver lobule.

Source : Neste Oxo AB Stenungsund

(177)

Type : Biochemical or cellular interactions

Remark : The in vitro inhibitory response of mouse and rat liver cytosolic glutathione S-transferase (GST) activities using the substrates 1,2-dichloro-4-nitrobenzene (DCNB) and 1,2-epoxy-3-(p-nitrophenoxy)-propane (ENPP) was determined for 2-ethylhexanol. The inhibitory effect of 2-ethylhexanolturned out to be weak.

Source : Neste Oxo AB Stenungsund

(178)

Type : Biochemical or cellular interactions

Remark : 2-Ethylhexanol was administered at 1% (w/w) in the diet to male C57BL/6 mice (details not reported). A slight increase in hepatic cytosolic (but not microsomal) epoxide hydrolase activitiy was detected.

Source : Neste Oxo AB Stenungsund

(179)

Type : Biochemical or cellular interactions

Remark : Up to 0.5 mM 2-ethylhexanol was added to primary rat hepatocyte cultures and the effect on peroxisomal enzyme activity was determined. Ethylhexanol had no effect on CN-insensitive palmitoyl-CoA oxidation (a peroxisomal marker).

Source : Neste Oxo AB Stenungsund

(180)

Type : Biochemical or cellular interactions

Remark : Male rats were fed the plasticisers di-(2-ethylhexyl)-phthalate (DEHP), di-(2-ethylhexyl)adipate (DEHA), di-

(2-ethylhexyl)sebacate (DEHS), adipic acid, and diethyl-phthalate at a dietary concentration of 2 % for 3 weeks. Hepatic peroxisome proliferation in association with an increase in liver size, increase in hepatic activities of the peroxisome-associated enzymes catalase and carnitine acetyltransferase, and hypolipidemia were observed in animals treated with DEHP, DEHA, and DEHS but not in animals fed adipic acid and diethylphthalate. To relate structure to biological activity, additional groups of rats were fed 2-ethylhexanol, hexanol, 2-ethylhexanoic acid, hexanoic acid, 2-ethylhexyl-aldehyde, hexylaldehyde, and 2-ethylhexylamine at a 2 % dose level. The changes induced by 2-ethylhexanol and 2-ethylhexanoic acid were comparable to those induced by DEHP, DEHA, and DEHS.

Source : Neste Oxo AB Stenungsund

(99)

Type : Biochemical or cellular interactions

Remark : Male F-344 rats were administered a diet containing 2 % (v/w) 2-ethylhexanol for 3 weeks. Then, serum triglyceride and cholesterol values were determined. A significant decrease in both serum cholesterol and triglyceride was found in animals treated with 2-ethylhexanol.

Source : Neste Oxo AB Stenungsund

(181)

Type : Biochemical or cellular interactions

Remark : The effects of exposure to 2-ethylhexanol on hepatic microsomal oxidation were investigated in male Sprague-Dawley rats. The metabolic clearance on antipyrine was utilized as an in vivo measure of the activity of the hepatic microsomal oxidative enzyme system. Subchronic (7 days) p.o. treatment of rats with 2-ethylhexanol produced a substancial increase in both wet liver weight and antipyrine clearance relative to corn oil-treated rats. Whereas subchronic treatment with 2-ethylhexanol produced apparent induction of hepatic microsomal oxidation enzymes, administration of a single dose was associated with immediate inhibition of the metabolism of antipyrine.

Source : Neste Oxo AB Stenungsund

(182)

Type : Biochemical or cellular interactions

Remark : 2-Ethylhexanol was administered by gavage for 14 days to male rats (Alderly Park Wistar-derived) at a dose equivalent to 1 mmol/kg/day. This dose was selected, because administration of DEHP produced hepatocellular tumors at 6000 ppm, a dose which approximates to 1 mmol/kg/day. It could be demonstrated, that 2-ethylhexanol did not induce testicular atrophy, hepatomegaly, peroxisome proliferation or hypolipidaemia, while DEHP did produce liver effects.

Source : Neste Oxo AB Stenungsund

(183)

Type : Biochemical or cellular interactions

Remark : Groups of six Sprague-Dawley rats were given five daily oral doses of 2.7 mmoles/kg body weight 2-ethylhexanol. No testicular damage was observed. In contrast, in animals which received corresponding oral doses of mono-(2-ethylhexyl)-phthalate the number of degenerated spermatocytes and spermatids was increased.

Source : Neste Oxo AB Stenungsund

(113)

Type : Biochemical or cellular interactions
Remark : The influence of several hepatotoxic chemicals, including 2-ethylhexanol, and hypoxia on phagocytic activity of Kupffer cells in perfused rat liver was investigated. A recently developed optical method was used to determine rates of phagocytosis of carbon articles by Kupffer cells in periportal and pericentral regions of the liver lobule based on changes in reflected light from the liver surface. With all chemicals studied, a rapid (10-30 min) decline in the rate of phagocytosis preceded parenchymal cell death as assessed from release of lactate dehydrogenase. These chemicals impaired parenchymal cell energy status as indicated by inhibition of oxygen uptake and bile flow prior to cell death.
Source : Neste Oxo AB Stenungsund

(184)

Type : Biochemical or cellular interactions
Remark : In order to investigate a proposed relationship between induction of hepatic microsomal lauric acid hydroxylase activity and peroxisome proliferaiton in the liver, male Wistar rats were treated with peroxisome proliferating compounds, and the lauric hydroxylase activity, the immunochemical detectabel levels of cytochrome P450 4A1 and the activities of peroxisomal enzymes were determined. 2-Ethylhexanol caused an induction of levels of P450 4A1 (3-fold), lauric acid omega-hydroxylase activity (3-fold) and the activity of peroxisomal palmitoyl-CoA oxidase (2-fold).
Source : Neste Oxo AB Stenungsund

(185)

Type : Biochemical or cellular interactions
Remark : Identification of the proximate peroxisome proliferator(s) derived from di-(2-ethylhexyl)-adipate has been achieved using primary hepatocyte cultures derived from different species and cyanide-insensitive fatty acetyl CoA oxidase (PCO) as a marker enzyme for peroxisome proliferation. In rat and mouse heaptocytes, the parent compound had no effect on peroxisomal beta-oxidation, but 2-ethylhexanol induced PCO activity 5-fold. No induction of peroxsomal beta-oxidation was observed in guinea pig and marmoset primary hepatocyte cultures.
Source : Neste Oxo AB Stenungsund

(186)

Type : Biochemical or cellular interactions
Remark : B6C3F1 mice received a diet with 1 % di(2-ethylhexyl)-adipate for 4 weeks, followed by single gavage administration of 110 or 120 mg 14C-2-ethylhexanol per kg body weight. In the liver DNA, only trace amounts of radioactivity could be detected, which were deduced to be caused by the incorporation of metabolites of ethylhexanol. A similar result was obtained with rats. These were pretrerated for 4 weeks with 1% di(2-ethylhexyl)-phthalate in the diet and then received a single dose of 51 or 53 mg 14C-2-ethylhexanol /kg body weight.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(166)

Type : Biochemical or cellular interactions
Remark : The ability of 2-ethylhexanol to promote the development of putative preneoplastic lesions was evaluated. GGT+ foci were initiated in the livers of male Sprague-Dawely rats with a single dose of diethylnitrosamine following partial hepatectomy. Rats were fed a 2-ethylhexanol (0.17%) containing diet for 10 weeks. The test material produced essentially no effect with regard to number of GGT+ foci, peroxisome proliferation or liver weight.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(167)

Type : Biochemical or cellular interactions
Remark : The effect of 2-ethylhexanol on the dissociation of germinal cells from Sertoli cells in cultures of seminiferous tubule cell preparations was investigated. In contrast to mono-ethylhexyl-phthalate, a concentration of 26.1 ug/ml 2-ethylhexanol did not have a detectable effect on the germinal cell dissociation (incubation time was 48 hrs).
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(168)

Type : Biochemical or cellular interactions
Remark : Rats were fed ad libitum a diet containing 2% of 2-ethylhexanol for two weeks. At the end of this period the livers were removed, pieces were taken for electron microscopy, and the reminder was homogenized and subfractioned to obtain mitochondria and microsomes. Protein and various enzyme activities were measured. 2-Ethylhexanol did not have a detectable influence on peroxisomal palmitoyl -CoA oxidation, catalase, or urate oxidase, on mitochondrial protein content, cytochrome c oxidase, carnitine-acetyl transferase, or on microsomal protein content, cytochrome P-450 and NADPH-cytochrome c reductase.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(169)

Type : Biochemical or cellular interactions
Remark : Adult rat hepatocytes cultured for 48 h in the presence of 1 mM 2-ethylhexanol contained increased numbers of peroxisomes. The peroxisome proliferation was associated with a marked increase (9-fold) in the activity of carnitine acetyltransferase.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(170)

Type : Biochemical or cellular interactions
Remark : Primary rat hepatocyte cultures were used to compare the effects of some alkylphthalate esters on peroxisomal enzyme activities and morphology. Carnitine acteyltransferase activity in hepatocytes, treated with 1 mM (=130.2 ug/ml) 2-ethylhexanol for 48 hrs, was elevated 6-fold as compared

to the control.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(171)

Type : Biochemical or cellular interactions
Remark : 2-Ethylhexanol was fed to male Swiss-Webster mice at a concentration of 2 % in the diet for 10 days. Treatment resulted in increased absolute liver weights, increased cytosolic and microsomal epoxide hydrolase and GSH S-transferase activities, and an increased cytosolic and microsomal protein content of the liver, as compared to controls.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(172)

Type : Biochemical or cellular interactions
Remark : Kupffer cells, the resident hepatic macrophages, are activated by calcium and release a variety of mitogenic growth factors that may modulate cell proliferation. In this study, the cytosolic free calcium concentration in Fura-2-loaded cultured Kupffer cells was increased significantly following incubation with Wy-14,643 (1.25 mM), while equimolar concentrations of 2-ethylhexanol had no effect. However, at higher concentraitons (3 nM), ethylhexanol also increased intracellular calcium.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(173)

Type : Biochemical or cellular interactions
Remark : The dose response relationship for peroxisome proliferation due to 2-ethylhexanol was investigated in male and female Alderley Park rats (Wistar-derived and Fischer 344) and mice (Swiss and B6C3F1). The animals were administered 2-ethylhexanol for 14 consecutive days at doses from 0 to 1.05 g/kg/day for rats and 0 to 1.75 g/kg/day for mice. At doses above 1.05 g/kg/day, 2-ethylhexanol was toxic to male and female rats, leading to death of the animals. Relative liver weights were increased in a dose-related manner in both species and sexes examined. Essentially linear dose-response relationships were observed for the induction of peroxisomal beta-oxidation (measured as palmitoyl CoA oxidation activities) in rats and mice.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(174)

Type : Biochemical or cellular interactions
Remark : Toxicity of 2-ethylhexanol was assessed in the perfused rat liver. Livers from starved rats were perfused with 2-ethylhexanol (3 mM) dissolved in O2/CO2-saturated buffer. Following infusion of ethylhexanol, O2 uptake and ketone body formation were diminished by 50 and 80%, respectilely, and cell damage, as assessed by the appearance of lactate dehydrogenase in the effluent perfusate, was apparent. Only O2-rich upstream regions of the liver lobule were damaged as

reflected by trypan blue uptake. It is concluded, that the toxicity of ethylhexanol in the liver is dependent on local O2 tension and mitochondria are primary targets.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(175)

Type : Biochemical or cellular interactions
Remark : 2-Ethylhexanol (70uM) stimulated oxygen uptake in the perfused rat liver by about 10 % during the first 10 min of infusion. Perfusions with a hepatotoxic dose of ethylhexanol (3 mM) led to a transient increase in oxygen uptake followed by a rapid inhibition of respiration of over 50 % in 10 min. Lactate dehydrogenase release, indicative of irreversible cell death, was detected in the effluent perfusate after 20 min. Within 10 min of perfusion, ethylhexanol decreased the ATP/ADP ratio from 2.5 to 0.9. Thus, marked decreases in hepatic energy state due to inhibition of respiration pereceded cell death. The effect of ethylhexanol on isolated mitochondria was also studied: ethylhexanol stimulated state-4 rates of respiration, diminished coupled rates of respiration, and decreased the P/O ratio in a dose-dependent manner. It also decreased the uptake of radiolabelled CaCl2 by isolated mitochondria 4- to 5-fold. It was hypothesized, that ethylhexanol initially uncouples oxidative phosphorylation leading to diminished ATP synthesis and collapse of ion gradients across the mitochondrial membrane.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(176)

Type : Biochemical or cellular interactions
Remark : 2-Ethylhexanol causes toxicity exclusively to periportal regions of the perfused liver. To determine whether this toxicity was due to local oxygen tension or to drug delivery, isolated cylinders (plugs) of periportal and pericentral regions of the liver lobule from rats pretreated with phenobarbital were collected. Incubation of plugs with 2-ethylhexanol (0.1 to 4 mM) diminished urea synthesis in a dose-related manner and caused extensive cell damage. Plugs isolated from both regions of the liver lobule were affected similarly by ethylhexanol and O2. The data indicate, that ethylhexanol toxicity is dependent on oxygen tension in isolated sublobular regions of the liver lobule.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(177)

Type : Biochemical or cellular interactions
Remark : The in vitro inhibitory response of mouse and rat liver cytosolic glutathione S-transferase (GST) activities using the substrates 1,2-dichloro-4-nitrobenzene (DCNB) and 1,2-epoxy-3-(p-nitrophenoxy)-propane (ENPP) was determined for 2-ethylhexanol. The inhibitory effect of 2-ethylhexanolturned out to be weak.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(178)

Type : Biochemical or cellular interactions
Remark : 2-Ethylhexanol was administered at 1% (w/w) in the diet to male C57BL/6 mice (details not reported). A slight increase in hepatic cytosolic (but not microsomal) epoxide hydrolase activitiy was detected.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(179)

Type : Biochemical or cellular interactions
Remark : Up to 0.5 mM 2-ethylhexanol was added to primary rat hepatocyte cultures and the effect on peroxisomal enzyme activity was determined. Ethylhexanol had no effect on CN-insensitive palmitoyl-CoA oxidation (a peroxisomal marker).
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(180)

Type : Biochemical or cellular interactions
Remark : Male rats were fed the plasticisers di-(2-ethylhexyl)-phthalate (DEHP), di-(2-ethylhexyl)adipate (DEHA), di-(2-ethylhexyl)sebacate (DEHS), adipic acid, and diethyl-phthalate at a dietary concentration of 2 % for 3 weeks. Hepatic peroxisome proliferation in association with an increase in liver size, increase in hepatic activities of the peroxisome-associated enzymes catalase and carnitine acetyltransferase, and hypolipidemia were observed in animals treated with DEHP, DEHA, and DEHS but not in animals fed adipic acid and diethylphthalate. To relate structure to biological activity, additional groups of rats were fed 2-ethylhexanol, hexanol, 2-ethylhexanoic acid, hexanoic acid, 2-ethylhexyl-aldehyde, hexylaldehyde, and 2-ethylhexylamine at a 2 % dose level. The changes induced by 2-ethylhexanol and 2-ethylhexanoic acid were comparable to those induced by DEHP, DEHA, and DEHS.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(99)

Type : Biochemical or cellular interactions
Remark : Male F-344 rats were administered a diet containing 2 % (v/w) 2-ethylhexanol for 3 weeks. Then, serum triglyceride and cholesterol values were determined. A significant decrease in both serum cholesterol and triglyceride was found in animals treated with 2-ethylhexanol.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(181)

Type : Biochemical or cellular interactions
Remark : The effects of exposure to 2-ethylhexanol on hepatic microsomal oxidation were investigated in male Sprague-Dawley rats. The metabolic clearance on antipyrine was utilized as an in vivo measure of the activity of the hepatic microsomal oxidative enzyme system. Subchronic (7 days) p.o. treatment of rats with 2-ethylhexanol produced a

substancial increase in both wet liver weight and antipyrine clearance relative to corn oil-treated rats. Whereas subchronic treatment with 2-ethylhexanol produced apparent induction of hepatic microsomal oxidation enzymes, administration of a single dose was associated with immediate inhibition of the metabolism of antipyrine.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(182)

Type : Biochemical or cellular interactions
Remark : 2-Ethylhexanol was administered by gavage for 14 days to male rats (Alderly Park Wistar-derived) at a dose equivalent to 1 mmol/kg/day. This dose was selected, because administration of DEHP produced hepatocellular tumors at 6000 ppm, a dose which approximates to 1 mmol/kg/day. It could be demonstrated, that 2-ethylhexanol did not induce testicular atrophy, hepatomegaly, peroxisome proliferation or hypolipidaemia, while DEHP did produce liver effects.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(183)

Type : Biochemical or cellular interactions
Remark : Groups of six Sprague-Dawley rats were given five daily oral doses of 2.7 mmoles/kg body weight 2-ethylhexanol. No testicular damage was observed. In contrast, in animals which received corresponding oral doses of mono-(2-ethylhexyl)-phthalate the number of degenerated spermatocytes and spermatids was increased.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(113)

Type : Biochemical or cellular interactions
Remark : The influence of several hepatotoxic chemicals, including 2-ethylhexanol, and hypoxia on phagocytic activity of Kupffer cells in perfused rat liver was investigated. A recently developed optical method was used to determine rates of phagocytosis of carbon articles by Kupffer cells in periportal and pericentral regions of the liver lobule based on changes in reflected light from the liver surface. With all chemicals studied, a rapid (10-30 min) decline in the rate of phagocytosis preceded parenchymal cell death as assessed from release of lactate dehydrogenase. These chemicals impaired parenchymal cell energy status as indicated by inhibition of oxygen uptake and bile flow prior to cell death.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(184)

Type : Biochemical or cellular interactions
Remark : In order to investigate a proposed relationship between induction of hepatic microsomal lauric acid hydroxylase activity and peroxisome proliferaiton in the liver, male Wistar rats were treated with peroxisome proliferating compounds, and the lauric hydroxylase activity, the

immunochemical detectabel levels of cytochrome P450 4A1 and the activities of peroxisomal enzymes were determined. 2-Ethylhexanol caused an induction of levels of P450 4A1 (3-fold), lauric acid omega-hydroxylase activity (3-fold) and the activity of peroxisomal palmitoyl-CoA oxidase (2-fold).

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(185)

Type : Biochemical or cellular interactions
Remark : Identification of the proximate peroxisome proliferator(s) derived from di-(2-ethylhexyl)-adipate has been achieved using primary hepatocyte cultures derived from different species and cyanide-insensitive fatty acetyl CoA oxidase (PCO) as a marker enzyme for peroxisome proliferation. In rat and mouse heaptocytes, the parent compound had no effect on peroxisomal beta-oxidation, but 2-ethylhexanol induced PCO activity 5-fold. No induction of peroxsomal beta-oxidation was observed in guinea pig and marmoset primary hepatocyte cultures.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(186)

Type : Biochemical or cellular interactions
Remark : B6C3F1 mice received a diet with 1 % di(2-ethylhexyl)-adipate for 4 weeks, followed by single gavage administration of 110 or 120 mg 14C-2-ethylhexanol per kg body weight. In the liver DNA, only trace amounts of radioactivity could be detected, which were deduced to be caused by the incorporation of metabolites of ethylhexanol. A similar result was obtained with rats. These were pretrerated for 4 weeks with 1% di(2-ethylhexyl)-phthalate in the diet and then received a single dose of 51 or 53 mg 14C-2-ethylhexanol /kg body weight.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(166)

Type : Biochemical or cellular interactions
Remark : The ability of 2-ethylhexanol to promote the development of putative preneoplastic lesions was evaluated. GGT+ foci were initiated in the livers of male Sprague-Dawely rats with a single dose of diethylnitrosamine following partial hepatectomy. Rats were fed a 2-ethylhexanol (0.17%) containing diet for 10 weeks. The test material produced essentially no effect with regard to number of GGT+ foci, peroxisome proliferation or liver weight.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(167)

Type : Biochemical or cellular interactions
Remark : The effect of 2-ethylhexanol on the dissociation of germinal cells from Sertoli cells in cultures of seminiferous tubule

cell preparations was investigated. In contrast to mono-ethylhexyl-phthalate, a concentration of 26.1 ug/ml 2-ethylhexanol did not have a detectable effect on the germinal cell dissociation (incubation time was 48 hrs).

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(168)

Type : Biochemical or cellular interactions
Remark : Rats were fed ad libitum a diet containing 2% of 2-ethylhexanol for two weeks. At the end of this period the livers were removed, pieces were taken for electron microscopy, and the reminder was homogenized and subfractioned to obtain mitochondria and microsomes. Protein and various enzyme activities were measured. 2-Ethylhexanol did not have a detectable influence on peroxisomal palmitoyl -CoA oxidation, catalase, or urate oxidase, on mitochondrial protein content, cytochrome c oxidase, carnitine-acetyl transferase, or on microsomal protein content, cytochrome P-450 and NADPH-cytochrome c reductase.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(169)

Type : Biochemical or cellular interactions
Remark : Adult rat hepatocytes cultured for 48 h in the presence of 1 mM 2-ethylhexanol contained increased numbers of peroxisomes. The peroxisome proliferation was associated with a marked increase (9-fold) in the activity of carnitine acetyltransferase.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(170)

Type : Biochemical or cellular interactions
Remark : Primary rat hepatocyte cultures were used to compare the effects of some alkylphthalate esters on peroxisomal enzyme activities and morphology. Carnitine acteyltransferase activity in hepatocytes, treated with 1 mM (=130.2 ug/ml) 2-ethylhexanol for 48 hrs, was elevated 6-fold as compared to the control.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(171)

Type : Biochemical or cellular interactions
Remark : 2-Ethylhexanol was fed to male Swiss-Webster mice at a concentration of 2 % in the diet for 10 days. Treatment resulted in increased absolute liver weights, increased cytosolic and microsomal epoxide hydrolase and GSH S-transferase activities, and an increased cytosolic and microsomal protein content of the liver, as compared to controls.
Source : Neste Oxo AB Stenungsund

ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(172)

Type : Biochemical or cellular interactions
Remark : Kupffer cells, the resident hepatic macrophages, are activated by calcium and release a variety of mitogenic growth factors that may modulate cell proliferation. In this study, the cytosolic free calcium concentration in Fura-2-loaded cultured Kupffer cells was increased significantly following incubation with Wy-14,643 (1.25 mM), while equimolar concentrations of 2-ethylhexanol had no effect. However, at higher concentraitons (3 nM), ethylhexanol also increased intracellular calcium.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(173)

Type : Biochemical or cellular interactions
Remark : The dose response relationship for peroxisome proliferation due to 2-ethylhexanol was investigated in male and female Alderley Park rats (Wistar-derived and Fischer 344) and mice (Swiss and B6C3F1). The animals were administered 2-ethylhexanol for 14 consecutive days at doses from 0 to 1.05 g/kg/day for rats and 0 to 1.75 g/kg/day for mice. At doses above 1.05 g/kg/day, 2-ethylhexanol was toxic to male and female rats, leading to death of the animals. Relative liver weights were increased in a dose-related manner in both species and sexes examined. Essentially linear dose-response relationships were observed for the induction of peroxisomal beta-oxidation (measured as palmitoyl CoA oxidation activities) in rats and mice.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(174)

Type : Biochemical or cellular interactions
Remark : Toxicity of 2-ethylhexanol was assessed in the perfused rat liver. Livers from starved rats were perfused with 2-ethylhexanol (3 mM) dissolved in O2/CO2-saturated buffer. Following infusion of ethylhexanol, O2 uptake and ketone body formation were diminished by 50 and 80%, respectilely, and cell damage, as assessed by the appearance of lactate dehydrogenase in the effluent perfusate, was apparent. Only O2-rich upstream regions of the liver lobule were damaged as reflected by trypan blue uptake. It is concluded, that the toxicity of ethylhexanol in the liver is dependent on local O2 tension and mitochondria are primary targets.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(175)

Type : Biochemical or cellular interactions
Remark : 2-Ethylhexanol (70uM) stimulated oxygen uptake in the perfused rat liver by about 10 % during the first 10 min of

infusion. Perfusions with a hepatotoxic dose of ethylhexanol (3 mM) led to a transient increase in oxygen uptake followed by a rapid inhibition of respiration of over 50 % in 10 min. Lactate dehydrogenase release, indicative of irreversible cell death, was detected in the effluent perfusate after 20 min. Within 10 min of perfusion, ethylhexanol decreased the ATP/ADP ratio from 2.5 to 0.9. Thus, marked decreases in hepatic energy state due to inhibition of respiration pereceded cell death. The effect of ethylhexanol on isolated mitochondria was also studied: ethylhexanol stimulated state-4 rates of respiration, diminished coupled rates of respiration, and decreased the P/O ratio in a dose-dependent manner. It also decreased the uptake of radiolabelled CaCl2 by isolated mitochondria 4- to 5-fold. It was hypothesized, that ethylhexanol initially uncouples oxidative phosphorylation leading to diminished ATP synthesis and collapse of ion gradients across the mitochondrial membrane.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(176)

Type : Biochemical or cellular interactions
Remark : 2-Ethylhexanol causes toxicity exclusively to periportal regions of the perfused liver. To determine whether this toxicity was due to local oxygen tension or to drug delivery, isolated cylinders (plugs) of periportal and pericentral regions of the liver lobule from rats pretreated with phenobarbital were collected. Incubation of plugs with 2-ethylhexanol (0.1 to 4 mM) diminished urea synthesis in a dose-related manner and caused extensive cell damage. Plugs isolated from both regions of the liver lobule were affected similarly by ethylhexanol and O2. The data indicate, that ethylhexanol toxicity is dependent on oxygen tension in isolated sublobular regions of the liver lobule.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(177)

Type : Biochemical or cellular interactions
Remark : The in vitro inhibitory response of mouse and rat liver cytosolic glutathione S-transferase (GST) activities using the substrates 1,2-dichloro-4-nitrobenzene (DCNB) and 1,2-epoxy-3-(p-nitrophenoxy)-propane (ENPP) was determined for 2-ethylhexanol. The inhibitory effect of 2-ethylhexanolturned out to be weak.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(178)

Type : Biochemical or cellular interactions
Remark : 2-Ethylhexanol was administered at 1% (w/w) in the diet to male C57BL/6 mice (details not reported). A slight increase in hepatic cytosolic (but not microsomal) epoxide hydrolase activitiy was detected.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)

Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(179)

Type : Biochemical or cellular interactions
Remark : Up to 0.5 mM 2-ethylhexanol was added to primary rat hepatocyte cultures and the effect on peroxisomal enzyme activity was determined. Ethylhexanol had no effect on CN-insensitive palmitoyl-CoA oxidation (a peroxisomal marker).
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(180)

Type : Biochemical or cellular interactions
Remark : Male rats were fed the plasticisers di-(2-ethylhexyl)-phthalate (DEHP), di-(2-ethylhexyl)adipate (DEHA), di-(2-ethylhexyl)sebacate (DEHS), adipic acid, and diethyl-phthalate at a dietary concentration of 2 % for 3 weeks. Hepatic peroxisome proliferation in association with an increase in liver size, increase in hepatic activities of the peroxisome-associated enzymes catalase and carnitine acetyltransferase, and hypolipidemia were observed in animals treated with DEHP, DEHA, and DEHS but not in animals fed adipic acid and diethylphthalate. To relate structure to biological activity, additional groups of rats were fed 2-ethylhexanol, hexanol, 2-ethylhexanoic acid, hexanoic acid, 2-ethylhexyl-aldehyde, hexylaldehyde, and 2-ethylhexylamine at a 2 % dose level. The changes induced by 2-ethylhexanol and 2-ethylhexanoic acid were comparable to those induced by DEHP, DEHA, and DEHS.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(99)

Type : Biochemical or cellular interactions
Remark : Male F-344 rats were administered a diet containing 2 % (v/w) 2-ethylhexanol for 3 weeks. Then, serum triglyceride and cholesterol values were determined. A significant decrease in both serum cholesterol and triglyceride was found in animals treated with 2-ethylhexanol.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(181)

Type : Biochemical or cellular interactions
Remark : The effects of exposure to 2-ethylhexanol on hepatic microsomal oxidation were investigated in male Sprague-Dawley rats. The metabolic clearance on antipyrine was utilized as an in vivo measure of the activity of the hepatic microsomal oxidative enzyme system. Subchronic (7 days) p.o. treatment of rats with 2-ethylhexanol produced a substancial increase in both wet liver weight and antipyrine clearance relative to corn oil-treated rats. Whereas subchronic treatment with 2-ethylhexanol produced apparent induction of hepatic microsomal oxidation enzymes,

administration of a single dose was associated with immediate inhibition of the metabolism of antipyrine.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(182)

Type : Biochemical or cellular interactions
Remark : 2-Ethylhexanol was administered by gavage for 14 days to male rats (Alderly Park Wistar-derived) at a dose equivalent to 1 mmol/kg/day. This dose was selected, because administration of DEHP produced hepatocellular tumors at 6000 ppm, a dose which approximates to 1 mmol/kg/day. It could be demonstrated, that 2-ethylhexanol did not induce testicular atrophy, hepatomegaly, peroxisome proliferation or hypolipidaemia, while DEHP did produce liver effects.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(183)

Type : Biochemical or cellular interactions
Remark : Groups of six Sprague-Dawley rats were given five daily oral doses of 2.7 mmoles/kg body weight 2-ethylhexanol. No testicular damage was observed. In contrast, in animals which received corresponding oral doses of mono-(2-ethylhexyl)-phthalate the number of degenerated spermatocytes and spermatids was increased.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(113)

Type : Biochemical or cellular interactions
Remark : The influence of several hepatotoxic chemicals, including 2-ethylhexanol, and hypoxia on phagocytic activity of Kupffer cells in perfused rat liver was investigated. A recently developed optical method was used to determine rates of phagocytosis of carbon articles by Kupffer cells in periportal and pericentral regions of the liver lobule based on changes in reflected light from the liver surface. With all chemicals studied, a rapid (10-30 min) decline in the rate of phagocytosis preceded parenchymal cell death as assessed from release of lactate dehydrogenase. These chemicals impaired parenchymal cell energy status as indicated by inhibition of oxygen uptake and bile flow prior to cell death.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(184)

Type : Biochemical or cellular interactions
Remark : In order to investigate a proposed relationship between induction of hepatic microsomal lauric acid hydroxylase activity and peroxisome proliferaiton in the liver, male Wistar rats were treated with peroxisome proliferating compounds, and the lauric hydroxylase activity, the

immunochemical detectabel levels of cytochrome P450 4A1 and the activities of peroxisomal enzymes were determined.
2-Ethylhexanol caused an induction of levels of P450 4A1 (3-fold), lauric acid omega-hydroxylase activity (3-fold) and the activity of peroxisomal palmitoyl-CoA oxidase (2-fold).

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(185)

Type : Biochemical or cellular interactions
Remark : Identification of the proximate peroxisome proliferator(s) derived from di-(2-ethylhexyl)-adipate has been achieved using primary hepatocyte cultures derived from different species and cyanide-insensitive fatty acetyl CoA oxidase (PCO) as a marker enzyme for peroxisome proliferation. In rat and mouse heaptocytes, the parent compound had no effect on peroxisomal beta-oxidation, but 2-ethylhexanol induced PCO activity 5-fold. No induction of peroxsomal beta-oxidation was observed in guinea pig and marmoset primary hepatocyte cultures.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(186)

Type : Metabolism
Remark : 2-Ethylhexanol was efficiently absorbed following oral administration to rats. 14C associated with 2-ethyl[1-14C]-hexanol was rapidly excreted in respiratory CO2 ((6-7%), faeces (8-9%) and urine (80-82%), with essentially complete elimination by 28 h after administration.
The amount of label recovered in CO2 matched the amount of unlabelled 2-heptanone plus 4-heptanone recovered from urine, suggesting that both types of metabolites may have been derived from the major urinary metabolite, 2-ethylhexanoix acid, by decarboxylation following partial beta-oxidation. The 14CO2 appeared not to be derived from acetate or by reductive decarboxylation.
Other identified metabolites were 2-ethyl5-hydroxyhexanoic acid, 2-ethyl-5-ketohexanoic acid, and 2-ethyl-1,6-hexene-dioic acid. Only about 3% of the ethylhexanol was excreted unchanged.
Ethylhexanol was a competitive inhibitor of yeast alcohol dehydrogenase, but a good substrate for horse alcohol dehydrogenase.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(187)

Type : Metabolism
Remark : From experiments with perfused livers from starved rats it

is concluded that 2-ethylhexanol is oxidized via phenobarbital-inducible pathways to metabolites which do not inhibit ketogenesis and that ethylhexanol inhibits beta-oxidation of fatty acids in mitochondria but not in peroxisomes. Treatment of rats with ethylhexanol (0.32 g/kg i.p.) decreased plasma ketone bodies from 1.6 to 0.8 mM, increased hepatic triglycerides and increased lipid predominantly in periportal regions of the liver lobule.

Source : Neste Oxo AB Stenungsund

(188)

Type : Metabolism
Remark : Three rabbits were each given 3 ml of 2-ethylhexanol by gavage. Nearly 90% of ethylhexanol was excreted as alpha-ethylhexanoylglucuronide.
Source : Neste Oxo AB Stenungsund

(189)

Type : Metabolism
Remark : From experiments with perfused livers from starved rats it is concluded that 2-ethylhexanol is oxidized via phenobarbital-inducible pathways to metabolites which do not inhibit ketogenesis and that ethylhexanol inhibits beta-oxidation of fatty acids in mitochondria but not in peroxisomes. Treatment of rats with ethylhexanol (0.32 g/kg i.p.) decreased plasma ketone bodies from 1.6 to 0.8 mM, increased hepatic triglycerides and increased lipid predominantly in periportal regions of the liver lobule.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(188)

Type : Metabolism
Remark : Three rabbits were each given 3 ml of 2-ethylhexanol by gavage. Nearly 90% of ethylhexanol was excreted as alpha-ethylhexanoylglucuronide.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(189)

Type : Metabolism
Remark : From experiments with perfused livers from starved rats it is concluded that 2-ethylhexanol is oxidized via phenobarbital-inducible pathways to metabolites which do not inhibit ketogenesis and that ethylhexanol inhibits beta-oxidation of fatty acids in mitochondria but not in peroxisomes. Treatment of rats with ethylhexanol (0.32 g/kg i.p.) decreased plasma ketone bodies from 1.6 to 0.8 mM, increased hepatic triglycerides and increased lipid predominantly in periportal regions of the liver lobule.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(188)

Type : Metabolism
Remark : Three rabbits were each given 3 ml of 2-ethylhexanol by gavage. Nearly 90% of ethylhexanol was excreted as alpha-ethylhexanoylglucuronide.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(189)

Type : Toxicokinetics
Remark : Excretion balance studies were conducted in female Fischer 344 rats with high (500 mg/kg) and low (50 mg/kg) oral doses of [14C]2-ethylhexanol, and following repeated oral dosing at the low level. Dermal exposures were conducted for 6 hrs with a 1 g/kg applied dose of [14C]2-ethylhexanol. The bioavailability of unlabeled 2-ethylhexanol at 500 mg/kg was compared following oral dosing as a neat chemical, and an emulsion in aqueous Cremophore EL. The high, low and repeated low oral doses of 2-ethylhexanol showed similar excretion balance profiles of [14C], with some evidence of metabolic saturation at the high dose. No evidence of metabolic induction was seen following the repeated low oral dosing. All of the oral doses were eliminated rapidly, predominantly in the urine during the first 24 hr following dosing. The dosing resulted in only about 5% absorption of the 1 g/kg dose, with the majority of the dose recovered unabsorbed from the dermal exposure cell at 6 hr. The majority of the oral and dermal doses were eliminated as glucuronides of oxidized metabolites of 2-ethylhexanol. The major urinary metabolites detected were glucoronides of 2-ethyladipic acid, 2-ethylhexanoic acid, and 5-hydroxy-2-ethylhexanoic acid, and 6-hydroxy-2-ethylhexanoic acid. Only trace amounts of unchanged 2-ethylhexanol were seen in urine. The bioavailability of 2-ethylhexanol, as determined by pharmacokinetic analylsis of blood 2-ethylhexanoic acid levels, dosed orally as an emulsion in Cremophor EL, was found to be slightly, but not significantly, greater than 2-ethylhexanol dosed orally as a neat chemical.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(190)

Type : other
Remark : The hypotensive effect of 2-ethylhexanol was tested in rabbits and dogs. 0.002 to 0.032 mmoles/kg 2-ethylhexanol, injected i.v. into Vena jugularis or Vena femoralis, dose dependently decreased the blood pressure of rabbits.The heart rate increased considerably in direct relation to the dosage, as did the frequency of respiration. With dogs, no consistent hypotensive effects were observed.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(191)

5.11 EXPERIENCE WITH HUMAN EXPOSURE

Remark	:	No study located.
Source	:	Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Remark	:	Es liegen keine Untersuchungsberichte der BASF vor.
Source	:	BASF AG Ludwigshafen

(1) TRGS 900 (1993)

(2) Huels AG: Sicherheitsdatenblatt "2-Ethylhexanol", Version 11, 17 Feb. 1997

(3) Inhouse data from Neste Oxo AB, Stenungsund.

(4) Bundesminister des Innern (1996): Gemeinsames Ministerialblatt Nr. 16, 47. Jahrgang, 338, Kenn-Nr. 134 (29.04.1996)

(5) Stoerfall-Verordnung vom 20.09.1991

(6) Stoerfallverordnung (1991): Bundesgesetzblatt, Teil 1, Anhang II (28.09.1991)

(7) BASF AG, Sicherheitsdatenblatt 2-Ethylhexanol, 25.01.1996

(8) Hoechst AG (1996): EG-Sicherheitsdatenblatt 2-Ethylhexanol (17.06.1996)

(9) Celanese GmbH (1997): EG-Sicherheitsdatenblatt 2-Ethylhexanol (10.07.1997)

(10) Toxicological Evaluation of 2-Ethylhexanol (1993) Berufsgenossenschaft der chemischen Industrie, Heidelberg.

(11) Toxicological Evaluation of 2-Ethylhexanol (1992), Berufsgenossenschaft der chemischen Industrie, Heidelberg.

(12) Hoechst AG (1993): Sicherheitsdatenblatt 2-Ethylhexanol (23.05.1993)

(13) Hoechst AG (1993): Sicherheitsdatenblatt 2-Ethylhexanol (23.05.93)

(14) BASF AG, Sicherheitsdatenblatt 2-Ethylhexanol (28.01.94)

(15) BASF AG, Sicherheitsdatenblatt 2-Ethylhexanol (28.01.1994)

(16) Computer calculation from data in Boublik T et al, The vapor pressures of pure substances, Elsevier Scientific Publishing Company, New York 1973,p.419.

(17) BASF Sicherheitsdatenblatt, 2-Ethylhexanol (28.01.94)

(18) Huls Report, unpublished.

(19) Huls Report (unpublished)

(20) Neste Oxo AB, Vattenlöslighet 2-etylhexanol, 930621,1993 (unpublished)

(21) EPA (1990): EPA/OTS Doc. No. 869000000467 (original ref: List of available studies on 2-ethyl-1-hexanol.Huls America Inc. 1990-06-26)

(22) CHEMFATE database, April 1992.

(23) Safety Data Sheet ELF ATOCHEM Dec. 1990.

(24) Hoechst AG (1994): Interne Berechnung der Abt. UCV (17.05.94)

(25) Lyman, WJ, Reehl WF and Rosenblatt DH. (1981). Handbook of chemical property estimation methods. McGraw-Hill Book Co.; New York.

(26) Yasuhara et al (1981), Environ Sci Tech 15(5), 570-573

(27) Sheldon LS et al. (1978). Organic compounds in Delaware River. Envir Sci Tech 12, 1188.

(28) Cited in ECDIN database, Feb. 1992.

(29) Akiyama et al. 1980. Journal of the University of Occupational and Environmental Health 2-3, 285-300. (Cited in ECDIN database Feb. 1992)

(30) Pulak R and Madrid A. (1983). Envrion Sci Technol 17, 329-334.

(31) Francis AJ, et al. (1980). Nuclear Tech 50, 158-163.

(32) Lundgren A. (1989) Comparison of different models for environmental hazards classification of chemicals. The Swedish National Chemicals Inspectorate. Kemi Report No 9/89.

(33) Huels-report ST-42/91, 1991 (unpublished).

(34) EPA/OTS Doc. No. 869000000467 (original ref: List of available studies on 2-ethyl-1-hexanol. Huls America Inc. 1990-06-26)

(35) Hoechst AG (1980): Unpublished report (RWL 28.03.80)

(36) Hoechst AG (1980): Unveröffentl. Untersuchung (RWL 28.03.80)

(37) Hoechst AG (1979): Unveröffentl. Untersuchung (RWL 30.07.79)

(38) BASF AG (1989), Labor Oekologie: Unpublished report (88/0537) dated 28.02.89.

(39) BASF AG (1989), Labor Oekologie: Unveroeffentlichte Untersuchung (88/0537) vom 28.02.89

(40) Price KS et al.(1974). Brine shrimp bioassay and seawater BOD of petrochemicals. J of Wat Pollut Control Fed 46(1),63-77.

(41) Price KS, et al. (1974). Brine shrimp bioassay and sea-water BOD of petrochemicals. J Water Pollut Control Fed 46(1), 63-77

(42) Gaffney PE et al. 1976. Carpet and rug industry case study II: Biological effects. J water Pollut Control Fed 48, 2731-7.

(43) Method: Secondary effluent from municipal and industrial waste water treatment plants was used as seed (25-55 ml/l).

Results:	Municipal	Industrial
BOD5/COD	0.70	0.60
BOD10/COD	0.81	0.77
BOD20/COD	0.87	0.86

(44) Kmeto M and Batchelder TL. (1980). R & D Report, DOW Chemicals. Evaluation of 2-Ethylhexanol in the Aquatic Environment.August 11, 1980.

(45) Kmeto M and Batchelder TL. (1980). R & D Report, DOW Chemical. Evaluation of 2-Ethylhexanol in the Aquatic Environment. August 11, 1980.

(46) Loeb HA and Kelly WH. (1963). Acute oral toxicity of 1,496 chemicals force fed to carp. U.S. Fish Wildl Serv Sp Sci Report - Fish No 417, 1963.

(47) Geiger DL et al. (1985). Acute toxicities of organic chemicals to Fathead Minnows (Pimephales promelas), Vol.2 Centre for Environmental Studies, Univ. of Visconsin, USA.

(48) Dave G, et al. (1979). Biological effects of solvent extraction chemicals on aquatic organisms, J Chem Technol Biotechnol 29, 249-259

(49) Huels-Report F1202, 1991 (unpublished).

(50) Dave G and Lidman U. (1978). Biological and toxicological effects of solvent extraction chemicals range finding acute toxicity in the rainbow trout (Salmo gairderi Rich.) and in the rat (Rattus norwegicus L.). Hydrometallurgy 3, 210-216.

(51) Dave G, et al. (1979). Biological effects of solvent extraction chemicals on aquatic organisms, J Chem Technol Biotechnol 29, 249-257.

(52) Huls Report,(Unpublished).

(53) Kmeto M and Batchelder TL. (1980). R&D Report, DOW Chemicals. Evaluation of 2-Ethylhexanol in the Aquatic Environment. August 11, 1980.

(54) Devillers J, et al.(1987). A predictive structure-toxicity model with Daphnia magna. Chemosphere 16(6), 1149-1163.

(55) Dave G, et al. (1979). Biological effects of solvent extraction chemicals on aquatic organisms. J Chem Tech Biotechnol 29, 249-257.

(56) Huels Report AW-216, 1991 (unpublished).

(57) Huels-Report AW 174, 1988 (unpublished).

(58) Huls Report, (unpublished).

(59) Scala RA and Burtis EG. (1973). Acute toxicity of a homologous series of branched-chain primary alchohols. Am Industr Hygiene Assoc J 34, 439-499.

(60) Smyth HF, et al. (1969). Range-finding toxicity data: List VII. Am Indust Hygiene Assoc J 30, 470-476.

(61) Schmidt P, et al. (1974). Z Ges Hyg 20, 575-578.

(62) EPA Document No. 86-870001432, Microfische No. 0515594 (1962).

(63) EPA Document No. 86-870001383, Microfische No. OTS515545 (1940)

(64) Smyth HF, et al. (1969). Range-finding Toxicity Data: List VII. Am Ind Hyg Assoc J 30, 470-476.

(65) EPA Document No. 86-870001432, Microfiche No. OTS0515594 (1962).

(66) EPA Document No. 878210249, Microfische No. OTS0206260 (1981)

(67) Schmidt P, et al. (1974). Z Ges Hyg 20, 575-578

(68) Schmidt P, et al. (1974) Z Ges Hyg 20, 575-578.

(69) EPA Document No. 86-870001432, Microfische No. 0515594 (1962)

(70) EPA Document No. 86-870001383, Microfische No OTS515545 (1940)

(71) EPA Document No. 86-870001383, Michrofiche No. OTS515545 (1940).

(72) EPA document No. 86-890001535, Microfische No. OTS0520664 (1989).

(73) Scala RA and Burtis EG. (1973). Acute toxicity of a homologous series of branched- chain primary alcohols. Am Ind Hyg Assoc J 34, 493-499.

(74) Muller J and Greff G. (1984). Recherche du relation entre toxicite de molecules d'interet industriel et propietes physico-chimiques: test d'irritation des vois aeriennes superieurs applique à quatre familles chimique. Food Chem Toxicol 22, 661-668.

(75) Scala RA and Burtis EG. (1973). Acute toxicity of a homologous series of branched-chain primary alcohols. Am Ind Hyg Assoc J 34, 493-499.

(76) Hoechst AG (1951): Unpublished report (51.0049)

(77) Huls Report Nr 1046, 1987 (unpublished).

(78) Smyth HF, et al. (1969) Range-finding Toxicity Data: List VII. Am Ind Hyg Assoc J 30, 470-476.

(79) Schmidt P, et al. (1973). Zur Toxizität einiger C8-Aldhyde und Alkohole. Z Ges Hyg 19, 485-490.

(80) Schmidt P, et al. (1973). Zur Toxizität einiger C8-Aldehyde und Alkohole. Z Ges Hyg 19, 485-490.

(81) Hodge HC. (1943). Proc. Soc. Exptl. Biol. Med. 53, 20-23.

(82) Schmidt P, et al. (1973). Zur Toxizität einiger C8-Aldhyde und Alkohole Z Ges Hyg 19, 485-490.

(83) Huls Report No 1047,1987 (unpublished)

(84) Hoechst AG (1978). Unpublished report (78.0562)

(85) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, (87/631), 30.05.1988

(86) Hoechst AG (1978): Unpublished report (78.0562)

(87) Scala Ra and Burtis EG. (1973). Acute toxicity of a homologous series of branched-chain primary alcohols Am Ind Hyg Assoc J 34, 493-499.

(88) Huls Report No 1048, 1987 (unpublished).

(89) Smyth HF, et al. (1969) Range-finding Toxicity Data: List VII. Am Ind Hyg Assoc J 30, 470-476.

(90) EPA Document No. 88-920002733, Microfiche No. OTS0539492 (1992).

(91) Epstein WL (unpublished data) cited in: BIBRA, Toxicity Profile, 1987: 2-Ethyl-1-hexanol; (The British Industrial Biological Research Association)

(92) EPA Document No. 86-920001004, Microfiche No. OTS0536862 (1992).

(93) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 50I0044/89022, 16.04.1992

(94) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 36I0044/89001, 17.10.1990

(95) EPA Document No. 86-910000912, Michrofische No. OTS0529878 (1991).

(96) Moody DE and Reddy JK. (1978). Hepatic peroxisome (microbody) proliferation in rats fed plasticizers and related compounds. Toxicol Appl Pharmacol 45, 497-504.

(97) EPA Document No 86-870001426, Microfiche No. 0515588 (1980).

(98) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 10C0321/88022, 26.03.1991

(99) Moody DE and Reddy JK. (1978). Toxicol Appl Pharmacol 45, 497-504.

(100) EPA Document No. 86-8870000331, Microfiche No. OTS0516482 (1988).

(101) Hodgeson JR. (1987). Toxicol. Ind. Health 3(2), 49-61.

EPA Document No. 86-870000425; Microfiche No. OTS0513174 (1987)

(102) BASF (1991). Report on the oral toxicity of 2-Ethylhexanol in rats after the administration by gavage (aqueous emulsion) for three months. Project No. 31C0631/87077 (Cited in EPA OTS0529872.)

(103) Lake BG, et al. (1975). Studies on the hepatic effects of orally administered di-(2-ethylhexyl)phthalate in the rat. Toxicol Appl Pharmacol 32, 355-367.

(104) Sjöberg P, et al. (1986) Effects of di(2-ethylhexyl)phthalate and five of its metabolites in rat testis in vivo and in vitro. Acta Pharmachol Toxicol 58, 225-233.

(105) EPA Document No. 86-910000916, Microfiche No. OTS0529882 (1991).

(106) EPA Document No. 86-910000915, Microfiche No. OTS0529881 (1991).

(107) EPA Document No. 86-910000909, Microfiche No. OTS0529875 (1991)

(108) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 11C0631/87104, 26.03.1991

(109) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 11C0631/87102, 26.03.1991

(110) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 11C0631/87068, 26.03.1991

(111) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 31C0631/87077, 26.03.1991

(112) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 31C0631/87082, 26.03.1991

(113) Sjoeberg P, et al. (1986). Acta Pharmacol Toxicol 58, 225-233

(114) Schmidt P, et al. (1973). Zur Toxizität einiger C(-Aldehyde und Alkohole. Z Gesamt Hyg 19, 485-490.

(115) EPA Document No. 86-910000913, Microfiche No. OTS0529879 (1991).

(116) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 15C0321/88023, 26.03.1991

(117) EPA Document No. 86-910000908, Microfiche No. OTS0529874 (1991).

(118) BASF AG (1991). Report on the oral toxicity of 2-Ethylhexanol in mice after administration by gavage (aqueous emulsion) for three months. Project No 36C0631/87085 (Cited in EPA OTS0529876).

(119) EPA Document No. 86-910000914, Microfiche No. OTS0529880 (1991).

(120) EPA Document No. 86-910000917, Microfiche No. OTS0529883 (1991)

(121) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 16C0631/87105, 26.03.1991

(122) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 16C063/87103, 26.03.1991

(123) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 16C0631/87070, 26.03.1991

(124) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 36C0631/87085, 26.03.1991

(125) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 36C0631/87086, 26.03.1991

(126) Huls Report No 87/353, 1987 (unpublished).

(127) Zieger E, e al. (1985). Mutagenicity testing of di(2-ethylhexyl)phthalate and related chemiclas in Salmonella. Environ Mutagen 7, 213-232.

(128) Kirby PE, et al.(1982). Evaluation of di(2-ethylhexyl)phthalate and its major metabolites in the Ames test and L51 78Y mouse lymphoma mutagenicity assay. Environ Mutagen 4, 388-389.

(129) EPA Document No. 40-8226118, Microfiche No. OTS0508477 (1982).
EPA Document No. 86-870000939, Microfiche No. OTS0515377 (1982).
EPA Document No. 86-870001606, Microfiche No. OTS0516187 (1982).

(130) EPA Document No. 86-870000603, Microfiche No. OTS0515130 (1980).

(131) EPA Document No. 878213941, Microfiche No. OTS0206391 (1984)

(132) Agarwal DK, et al. (1985). J Toxicol Environ Health 16, 61-69.

(133) Shimizu H, et al. (1985). The results of microbial mutation test for forty-three industrial chemicals. Jpn J Ind Health 27, 400-419.

(134) Divincenzo GD, et al. (1985). Bacterial mutagenicity testing of urine from rats dosed with 2-ethylhexanol derived plasticizers. Toxicology 34, 247-259.

(135) EPA Document No. 86-870000603, Microfiche No. OTS0515130 (1981)

(136) Seed JL, et al. (1982). Mutagenic activity of phthalate esters in bacterial liquid suspension assay. Environ Health Perspect 45, 111-114.

(137) Tomita I, et al. (1982). Mutagenic/carcinogenic potential of DEHP and MEHP. Environ Health Perspect 45, 119-125.

(138) Phillips JB, et al.(1982). Genotoxicity studies of di(2-ethylhexyl)phthalate and its metabolites in CHO cells. Mutat Res 103, 297-304.

(139) Litton Bionetics Inc. (1985). Evaluation of 2-Ethylhexanol (2-EH) in the CHO/HGPRT forward mutation assay. No. PE-27.O-GT-LB.

(140) Kirby PE, et al. (1982). Evaluation of di(2-ethylhexyl)phthalate and its major metabolites in the Ames and L51 78Y mouse lymphoma mutagenicity assay. Environ Mutagen 4, 388-389.

(141) EPA Document No 86-870000603, Microfiche No OTS0515130 (1981).
Hodgson JR, et al. (1982). Environ Mutagen 4, 388.

(142) EPA Document No. 40-8226118, Microfiche No. OTS0508477 (1982).

(143) Ward JM, et al. (1986). Environ Health Perspect 65, 279-291.

(144) EPA Document No. 86-87000603, Microfiche No. OTS0515130 (1980)
Putman DL, et al. (1983). Cytogenetic evaluation of di(2-ethylhexyl)phthalate and its major metabolites in Fischer 344 rats. Environ Mutagen 5, 227-231.

(145) Rushbrook CJ, et al. (1982). Dominant lethal study of di(2-ethylhexyl)phthalate and its major metabolites in ICR/SIM mice. Environ Mutagen 4, 387.

(146) Valencia R, et al. (1985) Environ Mutagen 7, 325-348

(147) Valencia R, et al. (1985). Environ Mutagen 7, 325-348.

(148) EPA Document No. 86-870001604, Microfiche No. OTS0516185 (1982).
Barber ED, et al. (1985). The Toxicologist 5(1), 211.

(149) EPA Document No. 86-870001604, Microfiche No. OTS0516185 (1982)
Barber ED, et al. (1985). The Toxicologist 5(1), 211.

(150) CMA Oxo-Process Panel 2-ethylhexanol study summary, BASF (1992).
EPA Document No. 86-920000922, Microfiche No. OTS0535659 (1991).

(151) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 71C0622/88037, 24.01.1992

(152) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 99C0622/88045, 13.04.1992

(153) CMA Oxo-Process Panel 2-ethylhexanol study summary, BASF (1992).
EPA Document No. 86-920000922, Microfiche No. OTS0535659 (1991).
EPA Document No. 40-9211171, Microfiche No. OTS0540337 (1992).

(154) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 68C0622/88038, 20.12.1991

(155) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 99C0622/88049, 13.04.1992

(156) Nelson BK, et al. (1989). Developmental toxicicology evaluation of 1-Pentanol,1-Hexanol, and 2-Ethylhexanol administered by inhalation to rats. J AM Coll Toxicol 8; 405-410.

(157) BASF (1991). Study of prenatal toxicity of Isodecanol, 2-Ethylhexanol and 711 Alcohol (T.C.) in rats after oral administration (gavage). Project No. 92R0753/88069.
EPA Document No. 88-90000082, Microfiche No. OTS0524015 (1990)
EPA Document No. 8EHQ-0491-0910S, Microfiche No. OTS0524015-2 (1991).

(158) RitterEJ, et al. (1987). Teratogenicity of di(2-ethylhexyl)phthalate, 2-ethylhexanol , 2-ethylhexanoic acid and valproic acid and potentiation by caffeine. Teratology 35, 41-46.

(159) BASF AG: Abt. Toxikologie, unveroeffentlichte Untersuchung, Project No. 92R0753/88069, 21.03.1991

(160) Hardin BD, et al. (1987). Evaluation of 60 chemicals in a preliminary developmental toxicity test. Teratogenisis, Carcinogenisis, and Mutagenesis 7, 29-48

(161) Price CJ, et al. (1991). Teratology 43, 457 (Abstract No. P132).
Tyl RW, et al. (1991). Report No. RTI-307, Research Triangle Inst., Research Triangle Park,N.C., USA.

(162) Tyl RW, et al. (1992). The developmental toxicity of 2-ethylhexanol applied dermally to pregnant Fischer 344 rats. Fund Appl Toxicol 19, 176-185.

(163) EPA Document No. 86-900000345, Michrofiche No. OTS0522909 (1990)

(164) Barber ED, et al. (1992). Fund Appl Toxicol 19, 493-497

(165) Agarwal D, et al. (1982). Drug Metab Disp 10 (1), 77-80

(166) von Daeniken a, et al. (1984). Toxicol Appl Pharmacol 73, 373-387.

(167) DeAngelo AB, et al. (1986). Toxicology 41, 279-288.

(168) Gangolli SD. (1982). Environ Health Perspect 45, 77-84

(169) Ganning AE, et al. (1982). Achta Chem Scand 36, 563-565.

(170) Gray TJB, et al. (1982). Toxicol Lett 10, 273-279

(171) Gray TJB, et al. (1983). Toxicology 28, 167-179

(172) Hammock BD and Ota K. (1983) Toxicol Appl Pharmacol 71, 254-265

(173) Hijioka T, et al. (1991). Toxicol Lett 59, 239-244.

(174) Keith Y, et al. (1992). Arch Toxicol 66, 321-326

(175) Keller BJ, et al. (1990). J Pharmacol Exp Therap 252(3), 1355-1360.

(176) Keller BJ, et al. (1991). Toxicol Lett 57, 113-120

(177) Liang D, et al. (1991) Toxicol Appl Pharmacol 107, 344-349

(178) Law MYL and Moody DE. (1991) Toxic in Vitro 5 (3), 207-210

(179) Lundgren B, et al. (1988). Arch Toxicol Suppl 12, 288-293.

(180) Mitchell AM, et al. (1985). Toxicol Appl Pharmacol 80, 23-32

(181) Moody DE and Reddy JK. (1982). Toxicol Lett 10, 379-383.

(182) Pollack GM, et al. (1989). J Pharmacol Exp Therap 248(1), 176-181

(183) Rhodes C, et al. (1984). Toxicol Lett 21, 103-109

(184) teKoppele JM, et al. (1991). Toxicol Appl Pharmacol 110, 20-30.

(185) Dirven H A A M, et al. (1992). Biochem Pharmacol 43 (12), 2621-2629.

(186) Cornu MC, et al. (1992). Biochem Pharmacol 43(10), 2129-2134

(187) Albro PW (1975). Xenobiotica 5 (10), 625-636.

(188) Badr. MZ, et al. (1990). Biochem Pharmacol 39, 715-721

(189) Kamil IA, et al. (1953). Biochem J 53, 137-140.

(190) EPA Document No. 86-920000923, Michrofiche No. OTS0535660 (1992).

(191) Hollenbach K, et al. (1972). Z ges Hyg 7, 481-485

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 112-53-8
CAS No.	:	112-53-8
EINECS Name	:	dodecan-1-ol
EINECS No.	:	203-982-0
TSCA Name	:	1-Dodecanol
Molecular Formula	:	C12H26O

Producer Related Part

Company	:	EUROPEAN COMMISSION - European Chemicals Bureau
Creation date	:	11.02.2000

Substance Related Part

Company	:	EUROPEAN COMMISSION - European Chemicals Bureau
Creation date	:	11.02.2000
Memo	:	
Printing date	:	05.11.2001
Revision date	:	11.02.2000
Date of last Update	:	11.02.2000
Number of Pages	:	54
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	
Name	:	Aarhus Oliefabrik A/S
Partner	:	
Date	:	
Street	:	M.P. Bruunsgade 27
Town	:	8100 Aarhus C
Country	:	Denmark
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Type	:	
Name	:	Givaudan Roure SA
Partner	:	
Date	:	
Street	:	55, voie des Bans, BP 24
Town	:	95102 Argenteuil Cedex
Country	:	France
Phone	:	1/39 98 15 15
Telefax	:	1/39 82 00 15
Telex	:	
Cedex	:	

Type	:	
Name	:	Henkel KGaA
Partner	:	
Date	:	
Street	:	Henkelstr. 67
Town	:	40589 Duesseldorf
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Type	:	
Name	:	Huels AG
Partner	:	
Date	:	
Street	:	Postfach
Town	:	D-45764 Marl
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Type	:	
Name	:	Petrasol B.V.
Partner	:	
Date	:	
Street	:	P.O.Box 222
Town	:	4200 AE Gorinchem
Country	:	Netherlands
Phone	:	+31 183 630555
Telefax	:	+31 183 632272

Telex	:	23602 petr nl
Cedex	:	

Type	:	
Name	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Partner	:	
Date	:	
Street	:	Ueberseering 40
Town	:	22297 Hamburg
Country	:	Germany
Phone	:	040-6375-0
Telefax	:	040-6375-3496
Telex	:	21151320
Cedex	:	

Type	:	
Name	:	Sidobre Sinnova
Partner	:	
Date	:	
Street	:	Allee des Platanes
Town	:	77100 Meaux
Country	:	France
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

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	:	- % w/w

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

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

1-Dodecanol

Source	:	Sidobre Sinnova Meaux Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf Huels AG Marl

1-DODECANOL (ALTSTOFF)
Source : Henkel KGaA Duesseldorf

1-Dodecyl alcohol
Source : Henkel KGaA Duesseldorf

1-Dodekanol
Source : Henkel KGaA Duesseldorf

1-Hydroxydodecan
Source : Sidobre Sinnova Meaux
Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Huels AG Marl

1-Hydroxydodecane
Source : Henkel KGaA Duesseldorf

Adol 10
Source : Henkel KGaA Duesseldorf

Adol 11
Source : Henkel KGaA Duesseldorf

Adol 12
Source : Henkel KGaA Duesseldorf

Alcohol C-12
Source : Sidobre Sinnova Meaux
Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

Alcohol C12 lauric
Source : Givaudan Roure SA Argenteuil Cedex

Alfol 12
Source : Henkel KGaA Duesseldorf

ALKOHOL C12
Source : Huels AG Marl

C-12 Alkohol
Source : Henkel KGaA Duesseldorf

C12 Linear Primary Alcohol
Source : Henkel KGaA Duesseldorf

Cachalot L-50
Source : Henkel KGaA Duesseldorf

Cachalot L-90
Source : Henkel KGaA Duesseldorf

Conol 20P
Source : Henkel KGaA Duesseldorf

Dodecanol
Source : Sidobre Sinnova Meaux
Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

Dodecyl alcohol

Source : Sidobre Sinnova Meaux
Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

Dodecyl Alcohol
Source : Henkel KGaA Duesseldorf

Dodecylalcohol
Source : Sidobre Sinnova Meaux

Dodecylalkohol
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

Epal 1012
Source : Henkel KGaA Duesseldorf

Epal 12
Source : Henkel KGaA Duesseldorf

Epal 12/70
Source : Henkel KGaA Duesseldorf

Epal 12/85
Source : Henkel KGaA Duesseldorf

Epal 1214
Source : Henkel KGaA Duesseldorf

Epal 1218
Source : Henkel KGaA Duesseldorf

Epal 1412
Source : Henkel KGaA Duesseldorf

Exxal 12
Source : Henkel KGaA Duesseldorf

Hyfatol 12-70
Source : Aarhus Oliefabrik A/S Aarhus C

Kalcohl 20
Source : Henkel KGaA Duesseldorf

Laurex L1
Source : Henkel KGaA Duesseldorf

Laurex NC
Source : Henkel KGaA Duesseldorf

Lauric alcohol
Source : Henkel KGaA Duesseldorf

Lauric alcohol; Dodecyl alcohol
Source : ISIS/RISKLINE, release VI, 1997, Haskoning
Petrasol B.V. Gorinchem

Laurinic alcohol
Source : Sidobre Sinnova Meaux
Henkel KGaA Duesseldorf

Henkel KGaA Duesseldorf
Huels AG Marl

Laurol
Source : Sidobre Sinnova Meaux
Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

Lauryl 24
Source : Henkel KGaA Duesseldorf

Lauryl alcohol
Source : Aarhus Oliefabrik A/S Aarhus C

Lauryl Alcohol
Source : Henkel KGaA Duesseldorf

Lauryl alcohol (INCI)
Source : Henkel KGaA Duesseldorf

Laurylalcohol
Source : Sidobre Sinnova Meaux

Laurylalkohol
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Huels AG Marl
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

Lipocol L
Source : Henkel KGaA Duesseldorf

Lorol
Source : Henkel KGaA Duesseldorf

Lorol C 12
Source : Henkel KGaA Duesseldorf

MA-1214
Source : Henkel KGaA Duesseldorf

n-Dodecan-1-ol
Source : Sidobre Sinnova Meaux
Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Huels AG Marl
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

n-Dodecanol
Source : Sidobre Sinnova Meaux
Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Huels AG Marl
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

n-Dodecylalcohol
Source : Sidobre Sinnova Meaux

n-Dodecylalkohol

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Huels AG Marl

n-Dodekanol
Source : Henkel KGaA Duesseldorf

n-Laurylalcohol
Source : Sidobre Sinnova Meaux

n-Laurylalkohol
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Huels AG Marl

NAA 42
Source : Henkel KGaA Duesseldorf

Nacol 12
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

Pisol
Source : Henkel KGaA Duesseldorf

S 1298
Source : Henkel KGaA Duesseldorf

Sipol L 12
Source : Henkel KGaA Duesseldorf

Siponol 25
Source : Henkel KGaA Duesseldorf

Siponol L 2
Source : Henkel KGaA Duesseldorf

Siponol L 5
Source : Henkel KGaA Duesseldorf

1.3 IMPURITIES

1.4 ADDITIVES

1.5 QUANTITY

Production during the last 12 months :
Import during the last 12 months :
Quantity : 50 000 - 100 000 tonnes in

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.7 USE PATTERN

Type	:	type
Category	:	Non dispersive use
Type	:	type
Category	:	Wide dispersive use
Type	:	industrial
Category	:	Chemical industry: used in synthesis
Type	:	industrial
Category	:	Metal extraction, refining and processing of metals
Type	:	industrial
Category	:	Paints, lacquers and varnishes industry
Type	:	industrial
Category	:	Personal and domestic use
Type	:	industrial
Category	:	Public domain
Type	:	industrial
Category	:	Textile processing industry
Type	:	industrial
Category	:	other: metal processing industry
Type	:	use
Category	:	Cleaning/washing agents and disinfectants
Type	:	use
Category	:	Cosmetics
Type	:	use
Category	:	Flame retardants and fire preventing agents
Type	:	use
Category	:	Hydraulic fluids and additives
Type	:	use
Category	:	Intermediates
Type	:	use
Category	:	Lubricants and additives
Type	:	use
Category	:	Odour agents
Type	:	use
Category	:	Solvents

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit	:	MAK (DE)
Limit value	:	
Country	:	Germany
Remark	:	MAK-Wert: not established
Source	:	Huels AG Marl

(1)

1.9 SOURCE OF EXPOSURE

Memo	:	Emissionserklaerung Huels 1992
Remark	:	Release into the atmosphere on production site in 1992: less than 25 kg/a
Source	:	Huels AG Marl

(2)

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

Classified by	:	KBwS (DE)
Labelled by	:	KBwS (DE)
Class of danger	:	0 (generally not water polluting)
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(3)

Classified by	:	KBwS (DE)
Labelled by	:	
Class of danger	:	0 (generally not water polluting)
Remark	:	German Commission for the Assessment of Water Polluting Substances (Datasheet No. 656)
Source	:	Transfer program Henkel KGaA Duesseldorf

Classified by	:	KBwS (DE)
Labelled by	:	KBwS (DE)
Class of danger	:	0 (generally not water polluting)
Country	:	Germany
Remark	:	KBwS-Datenblatt 656
Source	:	Huels AG Marl

(4) (1)

1.14.2 MAJOR ACCIDENT HAZARDS

Legislation	:	Stoerfallverordnung (DE)
Substance listed	:	no
No. in directive	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

Legislation	:	Stoerfallverordnung (DE)
Substance listed	:	no
No. in directive	:	
Country	:	Germany
Source	:	Huels AG Marl

1.14.3 AIR POLLUTION

1.15 ADDITIONAL REMARKS

Source	:	Henkel KGaA Duesseldorf
Remark	:	TA Luft, Einstufung: Klasse 3 (Anhang E, Alkylalkohole) Wassergefaehrdungsklasse: WGK 0
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value : 19 - 23 ° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test substance : Laurylalcohol, > = 97% purity.

(5)

Value : = 23 - ° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(6)

Value : 23.7 - 23.9 ° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test substance : Laurylalcohol, chem. pure, > = 99,7% was tested.

(5)

Value : = 23.8 - ° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(7)

Value : = 24 - ° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(8)

Value : = 26 - ° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(9)

2.2 BOILING POINT

Value : = 264.6 - ° C at 1013 hPa
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(10)

Value : = 264.6 - ° C at 1013 hPa
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(10)

Value : = 264.6 - ° C at 1013 hPa
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(10)

Value : = 264.6 - ° C at 1013 hPa
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(10)

Value : = 264.6 - ° C at 1013 hPa

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(10)

Value : = 264.6 - ° C at 1013 hPa
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(10)

2.3 DENSITY

Type : density
Value : = .8309 - g/cm3 at 24° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(7)

Type : density
Value : .815 - .825 g/cm3 at 30° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test substance : Laurylalcohol, > = 97% purity.

(5)

Type : density
Value : = .822 - g/cm3 at 40° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(6)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .00022 - hPa at 20° C
Decomposition :
Method other (calculated): extrapoliert anhand Antoine-Gleichung
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(10)

Value : = .0087 - hPa at 20° C
Decomposition :
Method other (calculated): extrapoliert anhand Clausius-Clapeyronscher Gleichung
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(8)

Value : = .024 - hPa at 20° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(11)

Value	:	= 1.33 - hPa at 91° C
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(12)

2.5 PARTITION COEFFICIENT

Log pow	:	= 5.06 - at ° C
Method		other (calculated): Methode von Nys & Rekker
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(13)

Log pow	:	5.06 - at ° C
Method		other (calculated): Leo, Hansch: Version CLOG P 3.3
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(14)

Log pow	:	= 5.13 - at ° C
Method		other (measured): keine weiteren Angaben
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(15)

Log pow	:	= 5.36 - at ° C
Method		other (measured): HPLC
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	ambient temperature

(14)

2.6.1 WATER SOLUBILITY

Value	:	= 1.69 - mg/l at 16 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other: measured (ueber radioaktive Markierung)
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(16)

Value	:	1.9 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other: measured (GC)
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(17)

Value	:	= 2.7 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(18)

Value	:	= 2.9 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other: measured (keine weiteren Angaben)
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(13)

Value	:	= 3 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(19)

Value	:	= 4.28 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other: measured (ueber Oberflaechenspannung)
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(20)

Value	:	= 20 - mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(13)

Value	:	= 2.9 - mg/l at 34 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	other: measured (ueber radioaktive Markierung)
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(16)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	ca. 140 ° C
Type	:	open cup
Method	:	other: DIN 51758/ISO 2719
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test substance	:	Laurylalcohol, > = 97% purity.

(5)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

Result	:	non flammable
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

2.10 EXPLOSIVE PROPERTIES

Result	:	not explosive
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

2.11 OXIDIZING PROPERTIES

Result : no oxidizing properties
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

2.12 ADDITIONAL REMARKS

Remark : Dissoziationskonstante: pKa = 16.20 (geschaetzt; Methode nach Perrin, D.D. "pka Prediction for organic acids and bases" Chapman & Hall, London, 1981)
vermutlich Sekundaerzitat
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(14)

Remark : Geruch: angenehm blumenartig
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(21)

Remark : Viskositaet (40 Grad C): 9.7 mPa * s
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(22)

Remark : Geruchsschwelle: 2.2 +- 1.3 mg/m3
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(11)

Remark : Geruchsschwelle: 0.0255 mg/l
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(23)

Remark : Geruchsschwelle: 0.0000537 mg/l
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(24)

Remark : Odor: pleasant, like nuts
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(5)

Remark : Geruch: angenehm blumenartig
Source : Henkel KGaA Duesseldorf

(21)

Remark : Viskositaet (40 Grad C): 9.7 mPa * s
Source : Henkel KGaA Duesseldorf

(22)

Remark : Geruchsschwelle: 2.2 +- 1.3 mg/m3
Source : Henkel KGaA Duesseldorf

(11)

Remark : Geruchsschwelle: 0.0255 mg/l

Source : Henkel KGaA Duesseldorf

(23)

Remark : Geruchsschwelle: 0.0000537 mg/l
Source : Henkel KGaA Duesseldorf

(24)

Remark : Odor: pleasant, like nuts
Source : Henkel KGaA Duesseldorf

(5)

3.1.1 PHOTODEGRADATION

Remark	:	Adsorbiert an TiO2 wird Dodecanol (Konzentration ca. 37 mg/l) in waessriger Suspension bei Bestrahlung mit simuliertem Sonnenlicht in 2 bis 3 Stunden vollstaendig zu CO2 und H2O abgebaut
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(25)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	other: municipal sewage treatment plant effluent
Concentration	:	2mg/l related to Test substance related to
Contact time	:	
Degradation	:	79 - % after 29 day
Result	:	readily biodegradable
Kinetic of test substance	:	7 day = 54 - **%** 14 day = 68 - **%** 21 day = 80 - **%** - **%** - **%**
Deg. Product	:	
Method	:	Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	Nonylphenol 9.5 EO + 5 PO was used as solvent for poorly soluble test substance. Oxygen demand of solvent alone was determined and subtracted from oxygen demand of test substance plus solvent.

(26)

Type	:	aerobic
Inoculum	:	other: sewage treatment plant effluent/biological stage
Concentration	:	2mg/l related to related to
Contact time	:	
Degradation	:	79 - 58 % after 28 day
Result	:	readily biodegradable
Deg. Product	:	
Method	:	Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	EG-RiLi 84/449 Anh.V C4-E
Remark	:	ungenügender Restsauerstoff in der höheren Prüfkonzentration Lösungsvermittler eingesetzt
Source	:	Henkel KGaA Duesseldorf
Test condition	:	#1: 2 mg/l referring to Active Substance: 79% with parameter % BSB/CSB #2: 5 mg/l referring to Active Substance: 58% with parameter % BSB/CSB
Test substance	:	Active Matter = 100 %

(27) (28)

Type	:	aerobic
Inoculum	:	activated sludge, domestic
Concentration	:	100mg/l related to related to
Contact time	:	
Degradation	:	100 - % after 28 day
Result	:	other: readily degradable
Deg. Product	:	
Method	:	ISO Draft "BOD Test for insoluble substances"
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	two phase closed bottle test
Source	:	Henkel KGaA Duesseldorf
Test condition	:	#1: 100 mg/l referring to Chemical oxygen demand: 100% with parameter % BSB/CSB
Test substance	:	Active Matter = 100 %

(29) (30)

Type	:	aerobic
Inoculum	:	activated sludge, domestic, non-adapted
Concentration	:	100mg/l related to COD (Chemical Oxygen Demand) related to
Contact time	:	
Degradation	:	100 - % after 28 day
Result	:	
Kinetic of test substance	:	7 day = 72 - **%** 14 day = 89 - **%** 21 day = 93 - **%** - **%** - **%**
Deg. Product	:	
Method	:	ISO Draft "BOD Test for insoluble substances"
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Remark	:	Parameter: % BOD/COD
Source	:	Henkel KGaA Duesseldorf
Test condition	:	Direkteinwaage der Testsubstanz; kontinuierlich geschuettelt; 20 - 25 Grad C

(31)

Type	:	aerobic
Inoculum	:	predominantly domestic sewage, adapted
Contact time	:	
Degradation	:	23.2 - % after 5 day
Result	:	
Deg. Product	:	
Method	:	other: BOD-determination according to American Public Health Assoc. (1980), "Standard Methods for the Examination of Water and Wastewater"; 15th edition, S. 70ff.
Year	:	1980
GLP	:	
Test substance	:	
Remark	:	Einsatzkonz.: <= 3.2 mg/l ("never exceeded the water solubility of the chemical")
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	21 +- 3 Grad C

(32) (33)

Type	:	aerobic
Inoculum	:	activated sludge, domestic, non-adapted
Concentration	:	100mg/l related to COD (Chemical Oxygen Demand) related to
Contact time	:	
Degradation	:	100 - % after 28 day
Result	:	
Kinetic of test substance	:	7 day = 72 - % 14 day = 89 - % 21 day = 93 - % - % - %
Deg. Product	:	
Method	:	other: BOD-test for insoluble substances (BODIS-test). Closed bottle test (modification of RDA Blok test) with test substance as sole carbon source
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Parameter: % BOD/COD
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	Direkteinwaage der Testsubstanz; kontinuierlich geschuettelt; 20 - 25 Grad C

(31)

Type	:	aerobic
Inoculum	:	activated sludge, adapted
Contact time	:	
Degradation	:	15.2 - % after .3 day
Result	:	
Deg. Product	:	
Method	:	other: Warburg-Respirometer; method according to Bogan, R.H. & Sawyer, C.N., Sewage Ind. Wastes 26, 1069-1080 (1954)
Year	:	1954
GLP	:	
Test substance	:	

Remark	:	Einsatzkonz.: nicht angegeben Sauerstoffmangel durch Oberflaechenfilm?
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(34)

Type	:	aerobic
Inoculum	:	activated sludge, adapted
Contact time	:	
Degradation	:	29.7 - % after 5 day
Result	:	
Deg. Product	:	
Method	:	other: Warburg-Respirometer; method according to Bogan, R.H. & Sawyer, C.N., Sewage Ind. Wastes 26, 1069-1080 (1954)
Year	:	1954
GLP	:	
Test substance	:	
Remark	:	Einsatzkonz.: nicht angegeben
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	20 Grad C

(34)

Type	:	aerobic
Inoculum	:	domestic sewage
Contact time	:	
Degradation	:	27 - % after 5 day
Result	:	
Deg. Product	:	
Method	:	other: Warburg-Respirometer; method according to Bogan, R.H. & Sawyer, C.N., Sewage Ind. Wastes 26, 1069-1080 (1954)
Year	:	1954
GLP	:	
Test substance	:	
Remark	:	Einsatzkonz.: nicht angegeben
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	20 Grad C

(34)

Type	:	aerobic
Inoculum	:	other bacteria: Pseudomonas C12B
Contact time	:	
Degradation	:	ca. 100 - % after 2 day
Result	:	
Remark	:	Einsatzkonz.: nicht angegeben
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	30 Grad C; geschuettelt; Messparameter: Gas-Fluessig-Chromatographie, Dodecanol als einzige C-Quelle, Wert aus Graphik ermittelt.

(35)

Type	:	
Inoculum	:	other: no information
Contact time	:	
Degradation	:	20 - % after 5 day
Result	:	
Deg. Product	:	
Method	:	other: BOD-determination according to AFNOR-Guideline NF T90/103 (1969)
Year	:	1969

GLP :
Test substance :
Remark : Einsatzkonz.: nicht angegeben
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(36)

Type :
Inoculum : other bacteria: adapted microorganisms (no further details)
Concentration : 143mg/l related to Test substance
related to
Contact time :
Degradation : 75 - % after 1 day
Result :
Deg. Product :
Method : other: BOD-determination in a Warburg-Respirometer according to Leibnitz et al., Wasserwirtschaft-Wassertechnik 8, 410-416 (1958)
Year : 1958
GLP :
Test substance :
Remark : Sauerstoffmangel durch Oberflaechenfilm?
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(37)

Type :
Inoculum : other: adapted microorganisms (no further details)
Concentration : 143mg/l related to Test substance
related to
Contact time :
Degradation : 75 - % after 1 day
Result :
Deg. Product :
Method : other: BOD-determination in a Warburg-Respirometer according to Leibnitz et al., Wasserwirtschaft-Wassertechnik 8, 410-416 (1958)
Year : 1958
GLP :
Test substance :
Remark : Sauerstoffmangel durch Oberflaechenfilm?
Source : Henkel KGaA Duesseldorf

(37)

Type :
Inoculum : activated sludge, non-adapted
Concentration : 500mg/l related to Test substance
related to
Contact time :
Degradation : 13.4 - % after 1 day
Result :
Deg. Product :
Method : other: Warburg respirometer test
Year :
GLP :
Test substance :
Remark : Abbauversuche mit drei Belebtschlaemmen unterschiedlicher Herkunft; Sauerstoffmangel durch Oberflaechenfilm?
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 20 Grad C

(38)

Type :

Inoculum	:	other: no information
Contact time	:	
Degradation	:	32 - % after 5 day
Result	:	
Deg. Product	:	
Method	:	other: Warburg respirometer test
Year	:	
GLP	:	
Test substance	:	
Remark	:	Einsatzkonz.: nicht angegeben. Sauerstoffmangel durch Oberflaechenfilm?
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(39)

Type	:	
Inoculum	:	other bacteria: Pseudomonas sp. (adapted)
Concentration	:	800µmol/l related to Test substance related to
Contact time	:	
Degradation	:	ca. 78 - % after 2 day
Result	:	
Remark	:	Alkohole (C10 - C18) als Gemisch geprueft; Einzel-Abbauraten aus GC-Peaks bestimmt; Abbau-Werte aus Graphik ermittelt
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	Inkubation in Minimalmedium mit Gemisch aus Alkoholen (C10, C12, C14, C16 & C18) in Konzentrationen zu je 0.8 mmol/l; geschuettelt; 30 Grad C

(40)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
LC50	:	= 1.01 -
Method	:	other: method according to US EPA Committee on Methods for Toxicity Tests with Aquatic Organisms
Year	:	1975
GLP	:	no data
Test substance	:	other TS: dodecanol, no indication about purity
Remark	:	Toxizitaet nur auf geloesten Anteil bezogen, nicht auf Nominalkonzentration. Analyse durch Gaschromatographie.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	25 Grad C; pH 7.5; Sauerstoffsaettigung > 60 %

(41) (17)

Type	:	flow through
Species	:	other: no data
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	No mortality was found at saturation concentration (1 mg/l at 20°C).
Source	:	Henkel KGaA Duesseldorf
Test condition	:	Flow-through test (5 l/h); concentration of test substance was maintained at >= 90% during test (as measured by GLC).

(42)

Type	:	
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
LC50	:	= 1.924 -
Method	:	other: calculated (QSAR-study)
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(43)

Type	:	
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	
Unit	:	mg/l
Analytical monitoring	:	
LC50	:	.39 - .98
Method	:	other: calculated (QSAR-study)
Year	:	
GLP	:	

Test substance	:	
Remark	:	Testdauer: nicht angegeben
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(44)

Type	:	
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
LC50	:	= .1855 -
Method	:	other: calculated (QSAR-study; US-EPA)
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(45)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC0	:	= 100 -
EC50	:	= 320 -
EC100	:	= 1000 -
Method	:	other: DIN 38412, Teil 11 (Bestimmung der Wirkung von Wasserinhaltsstoffen auf Kleinkrebse, Daphnia Kurzzeittest)
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Test method conforms with OECD-Guideline 202 A.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(46)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC0	:	100 -
EC50	:	320 -
EC100	:	1000 -
Method	:	other: DIN 38412, Teil 11 (Daphnia, acute toxicity test)
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method conforms with OECD Guide-line 202, part 1
Remark	:	Related to: Active Substance
Source	:	Henkel KGaA Duesseldorf
Test substance	:	Active Matter = 100 %

(47) (48)

Type	:	
Species	:	Nitocra spinipes (Crustacea)

Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC50	:	.8 - 1.2
Method	:	other: statischer Test mit Brackwasser aus der Ostsee ohne Belueftung
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	Salinitaet: 7 ppt; 20-22 Grad C; pH-Wert nicht eingestellt; Aceton als Loesevermittler (< 0.5ml/l; EC50 (96h): 16700 mg/l)

(49) (50)

Type	:	
Species	:	Nitocra spinipes (Crustacea)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC50	:	= 1 -
Method	:	other: statischer Test mit Brackwasser aus der Ostsee ohne Belueftung
Year	:	
GLP	:	
Test substance	:	
Remark	:	TWEEN 80 als Loesevermittler (100 mg/l; EC50 (96h)=5000 mg/l)
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	Salinitaet: 7 ppt; 20-22 Grad C; pH-Wert nicht eingestellt; TWEEN 80 als Loesevermittler (100 mg/l; EC50 (96h): 5000 mg/l)

(51)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Scenedesmus subspicatus (Algae)
Endpoint	:	growth rate
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC0	:	= .3 -
EC10	:	= .73 -
EC50	:	= .97 -
Method	:	other: Algen-Zellvermehrungshemmtest, DIN 38412, Teil 9
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Test method conforms with OECD-Guideline 201.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(52)

Species	:	Scenedesmus subspicatus (Algae)
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC0	:	.4 -
EC50	:	.62 -

Method	:	other: DIN 38412, Teil 9 (Algal growth inhibition test)
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method conforms with OECD Guide-line 201
Remark	:	ErC50(0-72h) = 2,6 mg/l. Prod. wurde in unverg. Ethanol gelöst u. die entspr. Volumina in die Testgefäße geg.. Der Alkohol wurde vor Zugabe d. Testmed. abgedunstet. Related to: Test substance
Source	:	Henkel KGaA Duesseldorf
Test substance	:	Active Matter = 99 %

(53) (54)

Species	:	Scenedesmus subspicatus (Algae)
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC0	:	.3 -
EC50	:	.97 -
EC10	:	.73 -
Method	:	other: DIN 38412, Teil 9 (Algal growth inhibition test)
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method conforms with OECD Guide-line 201
Remark	:	ErC50(24-72h) > 10 mg/l. Test sollte sicherheitshalber wiederholt werden, da ErC50 >> EbC50! Related to: Active Substance
Source	:	Henkel KGaA Duesseldorf
Test substance	:	Active Matter = 99,7 %

(55) (56)

Species	:	Scenedesmus subspicatus (Algae)
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC0	:	.1 -
EC50	:	> 10 -
	:	.28 -
Method	:	other: DIN 38412, Teil 9 (Algal growth inhibition test)
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method conforms with OECD Guide-line 201
Remark	:	ErC50(0-72h) > 10 mg/l. Related to: Test substance
Source	:	Henkel KGaA Duesseldorf
Test substance	:	Active Matter = 100 %

(57) (58)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type	:	aquatic
Species	:	Pseudomonas putida (Bacteria)
Exposure period	:	30 minute(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC0	:	> 10000 -

Method	:	other: DIN 38412, Teil 27 (respiration inhibition test)
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	10 000 mg/l was highest concentration tested. Test substance could not be completely suspended; particles remained in test solution.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	Test substance was directly weighed into test vessel, warmed to 45 degr C and treated with ultrasound for 5 minutes.

(59)

Type	:	
Species	:	Bacillus subtilis (Bacteria)
Exposure period	:	
Unit	:	
Analytical monitoring	:	
Remark	:	In gesaettigter waessriger Loesung trat gegenueber Sporen von Bacillus subtilis eine Keimungshemmung von 10 % auf. Versuchszeitraum nicht angegeben
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	37 Grad C; Methanol als Loesevermittler (< 0.2 M; keine Hemmung bei dieser Konz.)

(60) (61)

Type	:	
Species	:	Candida albicans (Fungi)
Exposure period	:	18 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
MIC	:	> 1000 -
Method	:	other: statischer Test
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	37 Grad C; geschuettelt; Ethanol als Loesevermittler (keine Konzentrationsangabe; Ethanol-Kontrollen mitgelaufen)

(62)

Type	:	
Species	:	Escherichia coli (Bacteria)
Exposure period	:	18 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
MIC	:	> 1000 -
Method	:	other: statischer Test
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	37 Grad C; geschuettelt; Ethanol als Loesevermittler (keine Konzentrationsangabe; Ethanol-Kontrollen mitgelaufen)

(62)

Type	:	
Species	:	Pseudomonas putida (Bacteria)
Exposure period	:	30 minute(s)

Unit	:	mg/l
Analytical monitoring	:	
EC0	:	10000 -
Method	:	other: DIN 38412, Teil 27 (Bacterial oxygen consumption test)
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method conforms with OECD Guide-line 209
Remark	:	LC0/EC0 entspricht der höchsten Prüfkonzentration Related to: Test substance
Source	:	Henkel KGaA Duesseldorf
Test substance	:	Active Matter = 99 %

(63) (64)

Type	:	
Species	:	Saccharomyces cerevisiae (Fungi)
Exposure period	:	72 hour(s)
Unit	:	
Analytical monitoring	:	
Remark	:	keine Toxizitaet bei einer Konzentration von 100 g/l
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	28 Grad C

(65)

Type	:	
Species	:	Staphylococcus aureus (Bacteria)
Exposure period	:	18 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
MIC	:	= 1000 -
Method	:	other: statischer Test
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	37 Grad C; geschuettelt; Ethanol als Loesevermittler (keine Konzentrationsangabe; Ethanol-Kontrollen mitgelaufen)

(62)

Type	:	
Species	:	Tetrahymena pyriformis (Protozoa)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC50	:	= 1.58 -
EC100	:	= 2 -
NOEC	:	= 1.15 -
Method	:	other: photometrische Messung der Zellwachstumshemmung
Year	:	
GLP	:	
Test substance	:	
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(66) (67)

Type	:	
Species	:	other bacteria: Clostridium botulinum
Exposure period	:	
Unit	:	mg/l
Analytical monitoring	:	

MIC	:	= 2.5 -
Method	:	other: static cell multiplication inhibition test according to Huhtanen, P.N., J. Milk Food Technol. 38, 762-763 (1975)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Testdauer: nicht angegeben
Source	:	Henkel KGaA Duesseldorf
Test condition	:	anaerobe Bedingungen; Zellvermehrung visuell bestimmt

(68)

Type	:	
Species	:	other bacteria: Clostridium botulinum
Exposure period	:	
Unit	:	mg/l
Analytical monitoring	:	
MIC	:	= 2.5 -
Method	:	other: statischer Zellvermehrungshemmtest nach Huhtanen, P.N., J. Milk Food Technol. 38, 762-763 (1975)
Year	:	
GLP	:	
Test substance	:	
Remark	:	Testdauer: nicht angegeben
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	anaerobe Bedingungen; Zellvermehrung visuell bestimmt

(68)

Type	:	
Species	:	other bacteria: Mycoplasma gallisepticum
Exposure period	:	144 hour(s)
Unit	:	mmol/l
Analytical monitoring	:	
NOEC	:	> .064 -
Method	:	other: statischer Zellvermehrungshemmtest
Year	:	
GLP	:	
Test substance	:	
Remark	:	keine Hemmung bei einer Konzentration von 0.064 mmol/l = 11.9 mg/l
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	37 Grad C; Ethanol als Loesevermittler (< 1 % v/v, eingesetzte Konz. nicht toxisch)

(69)

Type	:	
Species	:	other bacteria: Mycoplasma pneumoniae
Exposure period	:	144 hour(s)
Unit	:	mmol/l
Analytical monitoring	:	
Method	:	other: statischer Zellvermehrungshemmtest
Year	:	
GLP	:	
Test substance	:	
Remark	:	bei einer Konzentration von 0.064 mmol/l (11.9 mg/l) 17.2 % Wachstumshemmung
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	37 Grad C; Ethanol als Loesevermittler (< 1 % v/v, eingesetzte Konz. nicht toxisch)

(69)

Type	:	
Species	:	other bacteria: Streptococcus mutans
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC18	:	= 2.3 -
Method	:	other: statischer Zellvermehrungshemmtest
Year	:	
GLP	:	
Test substance	:	
Remark	:	nach 4 Stunden betrug die Hemmung 26 % im Vergleich zur unbehandelten Kontrolle
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	37 Grad C; Ethanol als Loesevermittler (keine Konzentrationsangabe, Kontrollen enthielten gleiche Menge Ethanol)

(70)

Type	:	
Species	:	other bacteria: Streptococcus mutans MT 5091
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
MIC	:	= 6.25 -
Method	:	other: statischer Zellvermehrungshemmtest
Year	:	
GLP	:	
Test substance	:	
Remark	:	MIC = minimale Hemmkonzentration
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	37 Grad C; Methanol als Loesevermittler (Konz. nicht angegeben, MIC nicht bestimmt); Zellwachstum visuell als Truebung bestimmt

(71)

Type	:	
Species	:	other bacteria: mixed culture (see remarks)
Exposure period	:	75 hour(s)
Unit	:	
Analytical monitoring	:	
Method	:	other: statischer, anaerober Test
Year	:	
GLP	:	
Test substance	:	
Remark	:	Bakterienspezies: Mischung aus fakultativ anaeroben saeurebildenden Bakterien (B. cereus, B. panthotenticus, B. coagulans, Ps. aeruginosa, Lactobacillus plantarum, Corynebacterium) bei einer Konzentration von 2.1 mg/l wurde 84 % relative Gasproduktion, bei 20.8 mg/l 70 % relative Gasproduktion gemessen
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	35 Grad C; zweimal taeglich geschuettelt; Messparameter: Gasproduktion (die toxische Wirkung wurde anhand der Reduktion der Gasproduktion gegenueber einer unbehandelten Kontrolle festgestellt)

(72)

Type	:	

Species	:	other fungi: Candida 107
Exposure period	:	3 day
Unit	:	g/l
Analytical monitoring	:	
EC100	:	< 83 -
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	30 Grad C; Kulturen geschuettelt

(73)

Type	:	
Species	:	other fungi: Candida tropicalis
Exposure period	:	24 hour(s)
Unit	:	g/l
Analytical monitoring	:	
EC0	:	> 83 -
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	30 Grad C; Kulturen geschuettelt

(73)

Type	:	
Species	:	other fungi: Saccharomyces carlsbergiensis
Exposure period	:	24 hour(s)
Unit	:	g/l
Analytical monitoring	:	
EC100	:	< 83 -
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	30 Grad C; Kulturen geschuettelt

(73)

Type	:	
Species	:	other fungi: see remarks
Exposure period	:	
Unit	:	
Analytical monitoring	:	
Method	:	other: test for inhibition of spore germination
Year	:	
GLP	:	
Test substance	:	
Remark	:	Species: no antifungal activity up to: Aspergillus niger 10000 mg/l (5 d; 28 degr. C; pH 5.6) Trichoderma viride 100 mg/l (") Trichophyton mentagrophytes * (") Myrotecium verrucaria * (") Candida albican 100 mg/l (20 h; 37 degr. C; pH 5.6) Mucor mucedo 1000 mg/l (") * antifungal activity at all concentrations tested (lowest tested concentration: 100 mg/l).
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test condition	:	petri dishes with Sabouraud agar containing test substance were inoculated with 1 drop of spore suspension (6 x 10 exp 6 spores/ml). Test substance was dissolved in dimethyl sulfoxide (no particulars on end concentration in test). Tested concentrations: 100, 1000 and 10000 mg/l.

(74)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species	:	Daphnia magna (Crustacea)
Endpoint	:	reproduction rate
Exposure period	:	21 day
Unit	:	mg/l
Analytical monitoring	:	no
NOEC	:	= 1 -
LCEC	:	= 3 -
Method	:	other: according to UBA-Verfahrensvorschlag: "Verlaengerter Toxizitaetstest bei Daphnia magna" (Stand: 1.2.1984)
Year	:	1984
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Most sensitive parameter: number of offspring/parent. Test method conforms with OECD-Guideline 202, Part 2.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(75)

Species	:	Daphnia magna (Crustacea)
Endpoint	:	
Exposure period	:	21 day
Unit	:	mg/l
Analytical monitoring	:	
NOEC	:	1 -
LCEC	:	3 -
Method	:	other: Daphnia-Life-Cycle-Test (UBA-Proposition February 1984)
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Method conforms with OECD Guide-line 202, part 2. Verlaengerter Toxizitaetstest bei Daphnia magna. Bestimmung der NOEC fuer Reproduktionsrate, Mortalitaet und den Zeitpunkt des ersten Auftretens von Nachkommen). UBA-Verfahrensvorschlag vom Februar...
Remark	:	Related to: Active Substance
Source	:	Henkel KGaA Duesseldorf
Test substance	:	Active Matter = 100 %

(76) (77)

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

Species	:	other terrestrial plant: Pinus strobus
Endpoint	:	
Exposure period	:	
Unit	:	
Remark	:	Dodecanol stimuliert die Keimung von Pollen der Pinie (Pinus strobus) in Konzentrationen bis 25 ul/l; bei 50 und 100 ul/l wird die Keimung leicht gehemmt.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(78)

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

Remark : Mueckentoxizitaet:
LD50 = 0.04 l/m2 (Eier von Aedes aegypti, 72 h)
LD90 = 0.07 l/m2 (Eier von Aedes aegypti, 72 h)
LD50 = 0.04 l/m2 (Eier von Aedes scutellaris, 72 h)
LD90 = 0.07 l/m2 (Eier von Aedes scutellaris, 72 h)
vergleichbare Werte bei Larven und Puppen
Angaben in l/m2 Wasseroberflaeche; 150 ml/Testansatz; T = 25-27 Grad C; 0.04 l/m2 = 1360 mg/l; 0.07 l/m2 = 2380 mg/l

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(79)

Remark : Mueckentoxizitaet:
Abtoetung aller eingesetzten Larven und Puppen von Culex quinquefasciatus in einem Versuchszeitraum von 48 h bei einer Konzentration von ca. 2.9 mg/l; T = 25 Grad C

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(80)

Remark : Assimilation durch Mikroorganismen:
Der Pseudomonas-Stamm C12B kann auf Dodecanol als einziger Kohlenstoffquelle wachsen.

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(81)

Remark : Virentoxizitaet:
30 min. Inkubation mit Testsubstanz bei Raumtemperatur;
Parameter: Reduktion der plaque-forming units.
Bacteriophage phi 6: EC50 = 0.007 mM (= 1.3 mg/l)
Bacteriophage phi 23-1-a: EC50 = > 1 mM (> 186.3 mg/l)

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(82)

Remark : Mit Dodecanol getraenkte Filterplaettchen hemmen das Wachstum von Pilzen (Candida albicans, Trichophyton mentagrophytes und rubrum, Epidermophyton floccosum) und in geringerem Ausmass von gram-negativen Bakterien (Pseudomonas aeruginosa, Escherichia coli). Keine Hemmung von gram-positiven Bakterien (Bacillus subtilis, Staphylococcus aureus).

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(83)

Remark : Toxizitaet gegenueber Kaulquappen (Rana temporaria): Dodecanol narkotisiert Kaulquappen von Rana temporaria ab einer Konzentration von 0.0075 mM = 1.4 mg/l (Parameter: Reflexbewegungen nach mechanischem Stimulus). Narkose ist reversibel.

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(84)

Remark : Toxizitaet gegenueber Kaulquappen (Spezies nicht angegeben): EC50 = 5.4 uM (1 mg/l). Parameter: Verlust des Gleichgewichtssinnes. Effekte sind reversibel.

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(85)

Remark : Mueckentoxizitaet:
Abtoetung aller eingesetzten Larven und Puppen von Culex quinquefasciatus in einem Versuchszeitraum von 48 h bei einer Konzentration von ca. 2.9 mg/l; T = 25 Grad C

Source : Henkel KGaA Duesseldorf

(80)

Remark : Assimilation durch Mikroorganismen:
Der Pseudomonas-Stamm C12B kann auf Dodecanol als einziger Kohlenstoffquelle wachsen.

Source : Henkel KGaA Duesseldorf

(81)

Remark : Virentoxizitaet:
30 min. Inkubation mit Testsubstanz bei Raumtemperatur; Parameter: Reduktion der plaque-forming units.
Bacteriophage phi 6: EC50 = 0.007 mM (= 1.3 mg/l)
Bacteriophage phi 23-1-a: EC50 = > 1 mM (> 186.3 mg/l)

Source : Henkel KGaA Duesseldorf

(82)

Remark : Mit Dodecanol getraenkte Filterplaettchen hemmen das Wachstum von Pilzen (Candida albicans, Trichophyton mentagrophytes und rubrum, Epidermophyton floccosum) und in geringerem Ausmass von gram-negativen Bakterien (Pseudomonas aeruginosa, Escherichia coli). Keine Hemmung von gram-positiven Bakterien (Bacillus subtilis, Staphylococcus aureus).

Source : Henkel KGaA Duesseldorf

(83)

Remark : Toxizitaet gegenueber Kaulquappen (Rana temporaria): Dodecanol narkotisiert Kaulquappen von Rana temporaria ab einer Konzentration von 0.0075 mM = 1.4 mg/l (Parameter: Reflexbewegungen nach mechanischem Stimulus). Narkose ist reversibel.

Source : Henkel KGaA Duesseldorf

(84)

Remark : Toxizitaet gegenueber Kaulquappen (Spezies nicht angegeben): EC50 = 5.4 uM (1 mg/l). Parameter: Verlust des Gleichgewichtssinnes. Effekte sind reversibel.

Source : Henkel KGaA Duesseldorf

(85)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 5000 - mg/kg bw
Method	:	other: Henkel-method "Acute oral toxicity"
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Limit-Test
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(86)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 5000 - mg/kg bw
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Limit-Test
Source	:	Henkel KGaA Duesseldorf

(87)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 3125 - mg/kg bw
Method	:	Directive 84/449/EEC, B.1 "Acute toxicity (oral)"
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA Duesseldorf

(88)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 30000 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Calculated from the dose originally given (36 ml/kg) and the

density (0.83).
Seven rabbits which survived a dose of 36 ml technical lauryl alcohol/kg body weight, demonstrated no significant gross or microscopic organ injury.

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(89)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC0
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 18 hour(s)
Value : ca. 1 - mg/l
Method : other: chamber
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : No deaths occurred in any of the exposed animals.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(90)

Type : LC50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time :
Method : other
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Ten animals were exposed by aspiration to ca. 600 mg/kg dodecanol, and were observed for max. 24 h prior to sacrifice. Nine rats died during the observation period, seven deaths occurring within 7-30 minutes. Cause of death reported as massive, extensive, severe pulmonary haemorrhage.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(91)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 8300 - mg/kg bw
Method : other: not specified

Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Calculated from the dose originally given (10 ml/kg) and the density (0.83).
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(89)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	highly irritating
EC classification	:	
Method	:	Draize Test
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Fifty percent lauryl alcohol was tested. The exposure time was 24 hours under occlusion.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(92)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	irritating
EC classification	:	
Method	:	other: Henkel-method "Acute skin irritation"
Year	:	1977
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	1-Dodecanol was applied in a concentration of 50% in vaseline.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(92)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	slightly irritating
EC classification	:	
Method	:	Directive 84/449/EEC, B.4 "Acute toxicity (skin irritation)"

Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA Duesseldorf

(88)

Species	:	guinea pig
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	not irritating
EC classification	:	
Method	:	other: patch test, semi-occlusive
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	1-Dodecanol was tested 50% in vaseline for 24 h. No skin irritation was observed.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(92)

Species	:	human
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	not irritating
EC classification	:	
Method	:	other: see Remarks
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Volunteers; 50 %ig; 24 h Contact time; occlusive
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(92)

Species	:	human
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	not irritating
EC classification	:	not irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1984
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA Duesseldorf

(93)

Species	:	other: hairless mouse
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	

Result	:	not irritating
EC classification	:	
Method	:	other: Henkel KGaA "Skin irritation in hairless mice"
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The substance was applied once.
Source	:	Henkel KGaA Duesseldorf

(88)

Species	:	other: hairless mouse
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	slightly irritating
EC classification	:	
Method	:	other: Henkel KGaA "Skin irritation in hairless mice"
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The substance was applied twice daily to the same area of skin and gently massaged into it.
Source	:	Henkel KGaA Duesseldorf

(88)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	slightly irritating
EC classification	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Three rabbits were dosed with 0.1 ml/unwashed of undiluted commercial Lauryl alcohol. Maximum average irritation scores were 9.3 at 1 h. Most scores returned to zero within 3-4 days, but in one animal 14 day were required.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(94)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	slightly irritating
EC classification	:	
Method	:	Draize Test
Year	:	1959
GLP	:	no

Test substance	:	other TS
Remark	:	The tested Dodecanol/Tetradecanol mixture exerts only very mild irritating effects on the eyes of rabbits that normally wouldn't justify a classification as "irritant to the eye". With respect to the fact that some fatty alcohols are irritating to the skin as well as irritating to the eye, Henkel has desided to label the C10-C14 fatty alcohols consistently with the R-phrases R 36/38.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test substance	:	Analogy! The product "Lorol spezial-Type 70" was tested. This product consists of 70% C12- and 30% C14-fatty alcohols.

(95)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	slightly irritating
EC classification	:	not irritating
Method	:	Draize Test
Year	:	
GLP	:	no data
Test substance	:	other TS
Remark	:	Maximum average irritation scores were 9.3 at 1 h. Most scores returned to zero within 3-4 days, but in one animal 14 day were required.
Source	:	Henkel KGaA Duesseldorf
Test substance	:	Analogy to Alcohols C12-14 (80206-82-2), containing 63-68 % C12- and 24-25 % C14-alcohol

(96)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	slightly irritating
EC classification	:	
Method	:	Draize Test
Year	:	1959
GLP	:	no
Test substance	:	other TS
Remark	:	The tested Dodecanol/Tetradecanol mixture exerts only very mild irritating effects on the eyes of rabbits.
Source	:	Henkel KGaA Duesseldorf
Test substance	:	Analogy! The product "Lorol spezial-Type 70" was tested. This product consists of 70% C12- and 30% C14-fatty alcohols.

(97)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	slightly irritating

EC classification	:	
Method	:	Draize Test
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA Duesseldorf

(88)

5.3 SENSITIZATION

Type	:	other: maximation test
Species	:	human
Number of animals	:	
Vehicle	:	
Result	:	not sensitizing
Classification	:	
Method	:	other: method not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	A maximation test was carried out on 25 volunteers using a 4 % concentration of lauryl alcohol in petrolatum. No case of sensitization was reported.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test substance	:	See remark.

(98)

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	oral feed
Exposure period	:	37 days
Frequency of treatment	:	permanent by diet
Post obs. period	:	
Doses	:	0, 100, 500, 2000 mg/kg bw/day
Control group	:	yes
NOAEL	:	= 100 - mg/kg bw
Method	:	other: OECD Combined Repeat dose and Reproductive/Developmental Toxicity Screening Test.
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	The NOEL given is for the reduction in mean white blood cell count. Further, some changes were observed in plasma free cholesterol. No other effects were seen in the macroscopic and histological examinations. The NOAEL may therefore be greater than 100 mg/kg bw/day.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test substance	:	99% Dodecanol from Sigma (# L 5375) was tested.

(99)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration	:	4, 20, 100, 500 and 2.500 ug per plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: Henkel-method "Salmonella typhimurium reverse mutation assay"
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The test sample was suspended in water using Tween 80 as surfactant. Toxic effects were observed at concentrations of >= 100 ug/plate. At 500 ug/plate the chemical was latal to the test strains.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(100)

Type	:	Ames test
System of testing	:	Salmonella typhimurium
Concentration	:	4, 20, 100, 500 and 2500 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: Henkel-method "Salmonella typhimurium reverse mutation assay"
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The test sample was suspended in water using Tween 80 as surfactant. Toxic effects were observed at concentrations of >= 100 ug/plate. At 500 ug/plate the chemical was latal to the test strains.
Source	:	Henkel KGaA Duesseldorf

(101)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538
Concentration	:	0.01-50 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: modified Ames test
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test substance	:	Dodecanol, 90% purity, from Wako Pure Chemicals was tested.

(102)

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538
Concentration	:	0.01, 0.05, 0.1, 0.5, 1, 5, 10, 50 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: modified Ames test
Year	:	
GLP	:	no data

Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA Duesseldorf
Test substance	:	Dodecanol, 90% purity, from Wako Pure Chemicals was tested.

(103)

5.6 GENETIC TOXICITY 'IN VITRO'

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	other: albino mice, CFW 1
Route of admin.	:	gavage
Exposure period	:	24, 48, and 72 hours
Doses	:	5000 mg/kg body weight
Result	:	
Method	:	OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	No statistically significant enhanced mean values of micronucleated cells in polychromatic erythrocytes were seen following oral doses of 5000 mg/kg body weight. No reduction in the ratio of polychromatic to normochromatic erythrocytes was seen.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(104)

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	other: albino mice, CFW 1
Route of admin.	:	gavage
Exposure period	:	24, 48, and 72 hours
Doses	:	5000 mg/kg body weight
Result	:	
Method	:	OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	No statistically significant enhanced mean values of micronucleated cells in polychromatic erythrocytes were seen following oral doses of 5000 mg/kg body weight. No reduction in the ratio of polychromatic to normochromatic erythrocytes was seen.
Source	:	Henkel KGaA Duesseldorf

(105)

5.7 CARCINOGENITY

Species	:	mouse
Sex	:	female
Strain	:	Swiss
Route of admin.	:	dermal
Exposure period	:	60 weeks
Frequency of treatment	:	3 x / week
Post. obs. period	:	no

Doses	:	After an initial dose of benz(a)anthracene, 20 ul of a mixture of 20 g Dodecanol in 100 ml Cyclohexanol per application.
Result	:	
Control group	:	no
Method	:	other: method not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Repeated skin application of dodecanol showed a probable weak activity in promoting skin tumors in female mice that had received an initiating dose of 7,12-dimethyl-benz(a)anthracene. The authors stated that the initiation dose of PAH alone is non-carcinogenic. After treatment with dodecanol there were two tumor bearing mice out of 30 initiated animals. The tumors appeared at 39 and 49 weeks. The topical application was moderate irritant.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(106)

Species	:	mouse
Sex	:	female
Strain	:	ICR
Route of admin.	:	dermal
Exposure period	:	440 days
Frequency of treatment	:	3 x week
Post. obs. period	:	
Doses	:	10 mg/animal/application
Result	:	
Control group	:	other: with and without PAH induction
Method	:	other: method not specified
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The conclusion of the authors seems to be farfetched with respect to the fact of almost identical tumor incidences in the B[a]P plus Dodecanol and the B[a]P only treated groups.
Result	:	No tumors were observed in the 50 mice recieving dodecanol. Of the animals recieving dodecanol and B[a]P, 27 papillomas occurred in a total of 21 animals, 13 mice with squamous cell carcinoma. In a control group treated with B[a]P alone, 26 papillomas were observed in 16 animals, 12 of these tumors being squamous cell carcinoma. The authors conclude that these results suggest a weak to moderate co-carcinogenic effect.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

(107)

Species	:	mouse
Sex	:	male/female
Strain	:	other: A/He
Route of admin.	:	i.p.
Exposure period	:	8 weeks
Frequency of treatment	:	3 injections/week
Post. obs. period	:	16 weeks
Doses	:	Total doses of 2.4 g/kg and of 12 g/kg were given.
Result	:	
Control group	:	yes
Method	:	other: Test for Carcinogenicity by Pulmonary Tumor Response

Year	:	1973
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Lung tumors were observed in 2/15 female mice in the high dose group, and in 2/15 males and in 3/13 females in the low dose group. The lung tumor rate was not statistically significant relative to either untreated or vehicle controls. No tumors were found in other organs examined.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test substance	:	Dodecanol was administered in 0.1 ml tricaprylin.

(108)

5.8 TOXICITY TO REPRODUCTION

Type	:	One generation study
Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	oral feed
Exposure period	:	14 days
Frequency of treatment	:	permanent by diet
Premating exposure period		
Male	:	14 days
Female	:	14 days
Duration of test	:	5 weeks
Doses	:	0, 100, 500, 2000 mg/kg bw/day
Control group	:	yes
NOAEL Parental	:	= 2000 - mg/kg bw
NOAEL F1 Offspr.	:	= 2000 - mg/kg bw
Method	:	other: Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	No effects were seen on reproductive or developmental parameters up to doses of 2000 mg/kg bw/day. 1-Dodecanol in the doses administered had no influence on body weight, weight gain, food consumption and food efficiency in the parental generation. Pregnancy rates were not statistically altered and there were no differences in the lengths of the gestation periods. No organ toxicity was observed in the females. There was no effect on the number of pups per litter, weight, sex ratio or mortality rate from days 1-5 after birth. Autopsy indicated no effect from 1-Dodecanol under the conditions of this experiment.
Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Test substance	:	99% Dodecanol from Sigma (# L 5375) was tested.

(109)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.10 OTHER RELEVANT INFORMATION

Type : Metabolism
Source : Henkel KGaA Duesseldorf

(110) (111) (112)

5.11 EXPERIENCE WITH HUMAN EXPOSURE

Remark : 51 subjects allergic to wool wax alcohols have been tested, according to the ICDRG-method (305 in vaseline). Scores were measured after 24, 48 and 72 h. 1-Dodecanol reacted in 9 cases with reaction grade ++ (Erytheme and Papeln or Infiltrate) and +++ (erytheme, infiltrate or rather papulovesicle). The authors conclude that free fatty alcohols and especially 1-Dodecanol play a major part with respect to allergic reactions caused by wool wax in subjects allergic to wool wax.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(113)

6. References

(1) Henkel KGaA: Sicherheitsdatenblatt "Lorol C12", Ausgabe 05 vom 20.11. 1996

(2) Huels AG: Emissionserklaerung 1992 (confidential)

(3) Katalog wassergefaehrdender Stoffe, Datenblatt Nr. 656

(4) EUCLID-Data Sheet Henkel KGaA vom 20.11.1992

(5) Safety data sheet Henkel KGaA

(6) Noweck, K. & Ridder, H., Ullmann""s encyclopedia of industrial chemistry, 5th ed., Vol. A10, VCH, Weinheim, 277-296 (1987)

(7) Henkel, Fettchem. Tabellen, 3. Aufl., Duesseldorf (1971)

(8) Stull, D.R., Ind. Eng. Chem. 39, 517-540 (1947)

(9) Windholz, M. et al., The Merck index, 10th ed., Merck & Co., Rahway, New Jersey, 3413 (1983)

(10) Boublik,T. et al., "The Vapour Pressures of Pure Substances", Elsevier Scientific Publishing Company, Amsterdam (1973)

(11) Pliska, V., Scientific Papers from Institute of Chemical Technology, Prague, Food Technol. 6, 37-46 (1962)

(12) Lide, D.R. (ed.), "CRC Handbook of Chemistry and Physics", 71st edition, CRC Press, Boca Raton (1990-1991)

(13) Yalkowsky, S.H. & Valvany, S.C., J. Pharm. Sci. 69, 912-922 (1980)

(14) Burkhard, L. P.; D. W. Kuehl & G. D. Veith, Chemosphere 14 (1985), 1551-1560

(15) Leo, A. et al., Chem. Rev. 71, 525, 599 (1971)

(16) Krause, F.P. & Lange, W., J. Phys. Chem. 69, 3171-3173 (1965)

(17) Veith, G.D. et al., In: Bishop et al. (ed.) Aquatic toxicology and hazard assessment. 6th Symposium, ASTM 802, Philadelphia, 90-97 (1983)

(18) Amidon, G.L. et al., J. Pharm. Sci. 63, 1858-1866 (1974)

(19) Wakita, K. et al., Chem. Pharm. Bull. 34, 4663-4681 (1986)

(20) Robb, I.D., Aust. J. Chem. 19, 2281-2284 (1966)

(21) Neumueller, O.-A., Roempps Chemie-Lexikon, 8. Aufl., Franckh""sche Verlagshandlung, Stuttgart, 996 (1981)

(22) Stache, H., Tensid-Taschenbuch, 2. Aufl., Carl Hanser Verlag, Muenchen (1981)

(23) Mullins, L.J., Ann. N.Y. Acad. Sci. 62, 247-276 (1955)

(24) Laffort, P., Arch. Sci. Physiol. 17, 75-105 (1963)

(25) Pellizzetti, E. et al., Ann. Chim. 80, 81-87 (1990)

(26) Henkel KGaA, unpublished data (Report No. RE 920247)

(27) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No. PE 920302

(28) Henkel KGaA, unpublished data, Final report RE920247

(29) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No. PE 910219

(30) Henkel KGaA, unpublished data, Final report RE 920025

(31) Henkel KGaA, unpublished data (Report No. RE 920025)

(32) Babeu, L. & Vaishnav, D.D., J. Ind. Microbiol. 2, 107-115 (1987)

(33) Vaishnav, D.D., Chemosphere 16, 695-703 (1987)

(34) Bogan, R.H. & Sawyer, C.N., Sewage Ind. Wastes 27, 917-928 (1955)

(35) Prochazka, G.J. & Payne, W.J., Appl. Microbiol. 13, 702-705 (1965)

(36) Dore, M. et al., La tribune de cebedeau 28, 3-11 (1975)

(37) Winter, W., Wasserwirtschaft-Wassertechnik 12, 265-271 (1962)

(38) Gerhold, R.M. & Malaney, G.W., J. Water Pollut. Control Fed. 38, 562-579 (1966)

(39) Marion (1966), Ph.D. Thesis, Ohio State Univ., Columbus (Univers. Microfilms No. 67-2488); zitiert in Swisher, R. D., Surfactant biodegradation, Marcel Dekker Inc., New York (1970)

(40) Williams, J. P. et al., Appl. Microbiol. 14, 156-160 (1966)

(41) Veith, G.D. et al., Can. J. Fish. Aquat. Sci. 40, 743-748 (1983)

(42) Andreatta, A. et al., Tecnologie Chimiche 2 (1982), 60-66

(43) Devillers, J. et al., Chemosphere 17, 1531-1537 (1988)

(44) Basak, S.C. & Magnuson, V.R., Anzneim.-Forsch. 33, 501-503 (1983)

(45) Fiedler, H. et al., Toxicol. Environ. Chem. 28, 167-188 (1990)

(46) Henkel KGaA, unpublished data (Report No. RE 920019)

(47) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No. PE910224

(48) Henkel KGaA, unpublished data, Final Report RE 920019

(49) Bengtsson, B.-E. & Tarkpea, M., Marine Poll. Bull. 14 (1983), 213-214

(50) Linden, E. et al., Chemosphere 8, 843-851 (1979)

(51) Bengtsson, B.-E. et al., Chemosphere 13 (1984), 613-622

(52) Henkel KGaA, unpublished data (Report No. RE 920200)

(53) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No. 9400107-10

(54) Henkel KGaA, unpublished data, Final Report R 9400362

(55) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No. PE920244

(56) Henkel KGaA, unpublished data, Final Report RE 920200

(57) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No. PE910220

(58) Henkel KGaA, unpublished data, Final Report RE 920042

(59) Henkel KGaA, unpublished data (Report No. R 9400236)

(60) Yasuda-Yasaki, Y. et al., J. Bacteriol 136, 484-490 (1978)

(61) Yasuda-Yasaki, Y., Spores 7, 113-116 (1978)

(62) Morris, J.A. et al., J. Am. Oil Chem. Soc. 56, 595-603 (1979)

(63) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No. 9300287-28

(64) Henkel KGaA, unpublished data, Final Report R 9400236

(65) Calero, F.C. et al., Microbios 53, 175-180 (1988)

(66) Schultz, T.W. et al., Bull. Environ. Contam. Toxicol. 44, 67-72 (1990)

(67) Schultz, T.W. et al., Ecotoxicol. Environ. Safety 19, 243-253 (1990)

(68) Huhtanen, C.N., J. Food Prot. 43, 195-196 & 200 (1980)

(69) Fletcher, R.D. et al., Antimicrob. Agents Chemother. 19, 917-921 (1981)

(70) Crout, R.J. et al., Arch. Oral. Biol. 27, 1033-1037 (1982)

(71) Hattori, M. et al., Chem. Pharm. Bull. 35, 3507-3510 (1987)

(72) Playne, M.J. & Smith, B.R., Biotechnol. Bioeng. 25, 1251-1265 (1983)

(73) Gill, C.O. & Ratledge, C., J. Gen. Microbiol. 72, 165-172 (1972)

(74) Gershon, H. & Shanks, L., J. Pharm. Sci. 69, 381-384 (1980)

(75) Henkel KGaA, unpublished data (Report No. RE 920095)

(76) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No. PE910221

(77) Henkel KGaA, unpublished data, Final Report RE 920095

(78) French, R.C. et al., J. Agricult. Food Chem. 27, 184-187 (1979)

(79) Sinniah, B., Trans. R. Soc. Trop. Med. Hyg. 77, 35-38 (1983)

(80) Lorenzen, G.A. & Meinke, W.W., Mosquito News 28, 230-232 (1968)

(81) Payne, W.J., Biotechnol. Bioeng. 5, 355-365 (1963)

(82) Snipes, W. et al., Antimicrob. Agents Chemother. 11, 98-104 (1977)

(83) Janssen, A.M. et al., Pharm. Weekbl., Sci. Ed. 6, 157-160 (1984)

(84) Meyer, K.H. & Hemmi, H., Biochem. Zeitschr. 277, 39-71 (1935)

(85) Pringle, M.J. et al., Mol. Pharm. 19, 49-55 (1979)

(86) Henkel KGaA, unpublished data, Archive No. 930, Kaestner, W.

(87) Henkel KGaA, unpublished data, Archive-No. R 9500185 (Pb Ks 930)

(88) Henkel KGaA, unpublished data, Archive-No. TBD 810149 (Pb Pr 366)

(89) Industrial Hygiene and Toxicology 2nd Ed. II, 1467 (1963)

(90) Ulrich, C., et al., Am. Industrial Hygiene J. 40, 633-636 (1979)

(91) Gerard, H., et al., Arch. Environ. Health 13, 457-461 (1966)

(92) Kaestner, W., J. Soc. Cosmet. Chem. 28, 741-754 (1977)

(93) Henkel KGaA, unpublished data, Archive-No. R 9601427

(94) The Procter & Gamble Company, Test articles J0171.01 and J0172.01, Rabbit Eye Irritation, 191-566 (1980)

(95) Potokar, M., Henkel KGaA, unpublished data, Report-No. 305 (1980)

(96) The Procter & Gamble Company, Test articles J0171.01 and J0172.01, Rabbit Eye Irritation, 191-566 (1980) (LIT 9925)

(97) Henkel KGaA, unpublished data, Archive-No. TBD 800119 (Pb Pr 305)

(98) Opdyke, D., Fd. Cosmet. Toxicol. 11 (1), 1095 (1973)

(99) Hansen, E., "Combined Repeat Dose and Reproductive /Developmental Toxicity Screening Test on 1-Dodecanol in Rats", Institut of Toxicology, Danish National Food Agency, IT 9211105 (1992)

(100) Wallat, S., Henkel KGaA, unpublished data, Archive No. 295 (1982)

(101) Henkel KGaA, unpublished data, Archive-No. TBD 820115 (Pb Wa 295)

(102) Shimizu, H., et al., Jpn. J. Ind. Health 27, 400-419 (1985)

(103) Shimizu, H., Suzuki, Y., Takemura, N., Goto, S., Matsushita, H., Jpn. J. Ind. Health. 27, 400-419 (1985)

(104) Banduhn, N., Henkel KGaA, unpublished data, Report No. 92162 (1992)

(105) Henkel KGaA, unpublished data, Archive-No. RT 920162

(106) Sice, J., Toxicol. Appl. Pharmacol. 9, 70-74 (1966)

(107) Van Duuren, B., et al., J. of the National Cancer Inst. 56, 1237-1242 (1976)

(108) Stoner, G., et al., Cancer Research 33, 3069-3085 (1973)

(109) Hansen, E., "Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test on 1-Dodecanol in Rats", Institut of Toxicilogy, Danish National Foo Agency, IT 9211105 (1992)

(110) Iwate, Yuhei ; et al.: Percutaneous absorption of aliphatic compounds, Cosmet. Toiletries 102 (2), 53-68 (1987)

(111) Miura, Y., Omega - and (omega-1)-hydroxylation of 1-dodecanol by frog liver microsomes Lipids 16 (10), 721-725, (1981)

(112) Williams, R.T.: Detoxication Mechanisms. The Metabolism and Detoxication of Drugs, Toxic Substances and Other Organic Compounds, 2nd ed. p.46. Chapman & Hall, Ltd. London, 1959

(113) Auth, R., Pevny, I., Gernot, P., Akt. Dermatol. 10, 215-220 (1984)

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 111-27-3
CAS No.	:	111-27-3
EINECS Name	:	hexan-1-ol
EINECS No.	:	203-852-3
Molecular Weight	:	56.67
Molecular Formula	:	C6H14O

Producer Related Part

Company	:	EUROPEAN COMMISSION - European Chemicals Bureau
Creation date	:	10.02.2000

Substance Related Part

Company	:	EUROPEAN COMMISSION - European Chemicals Bureau
Creation date	:	10.02.2000
Memo	:	
Printing date	:	05.11.2001
Revision date	:	10.02.2000
Date of last Update	:	10.02.2000
Number of Pages	:	36
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	
Name	:	Givaudan Roure SA
Partner	:	
Date	:	
Street	:	55, voie des Bans, BP 24
Town	:	95102 Argenteuil Cedex
Country	:	France
Phone	:	1/39 98 15 15
Telefax	:	1/39 82 00 15
Telex	:	
Cedex	:	

Type	:	
Name	:	Henkel KGaA
Partner	:	
Date	:	
Street	:	Henkelstr. 67
Town	:	40589 Duesseldorf
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Type	:	
Name	:	Huels AG
Partner	:	
Date	:	
Street	:	Postfach
Town	:	D-45764 Marl
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

Type	:	
Name	:	NALCO-EXXON ENERGY CHEMICALS
Partner	:	
Date	:	
Street	:	CADLAND RD.
Town	:	SO45 3NP HYTHE
Country	:	United Kingdom
Phone	:	01703 883 883
Telefax	:	01703 883 882
Telex	:	
Cedex	:	

Type	:	
Name	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Partner	:	
Date	:	
Street	:	Ueberseering 40
Town	:	22297 Hamburg
Country	:	Germany
Phone	:	040-6375-0
Telefax	:	040-6375-3496

Telex : 21151320
Cedex :

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 : - % w/w

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

1-Hexanol
Source : Henkel KGaA Duesseldorf

1-HEXANOL (ALTSTOFF)
Source : Henkel KGaA Duesseldorf

1-Hexyl alcohol
Source : Henkel KGaA Duesseldorf

1-Hydroxyhexan
Source : Henkel KGaA Duesseldorf

1-Hydroxyhexane
Source : Henkel KGaA Duesseldorf

Alcohol C6 hexylic
Source : Givaudan Roure SA Argenteuil Cedex

Amylcarbinol
Source : Henkel KGaA Duesseldorf

Capronalkohol
Source : Henkel KGaA Duesseldorf

Caproyl alcohol
Source : Henkel KGaA Duesseldorf

Epal 108
Source : Henkel KGaA Duesseldorf

Epal 6
Source : Henkel KGaA Duesseldorf

Epal 610

Source : Henkel KGaA Duesseldorf

Exxal 6
Source : Henkel KGaA Duesseldorf

FA-C6
Source : Henkel KGaA Duesseldorf

Hexan-1-ol
Source : Henkel KGaA Duesseldorf

Hexanol
Source : Henkel KGaA Duesseldorf

Hexyl Alcohol
Source : Henkel KGaA Duesseldorf

hexyl alcohol
Source : Huels AG Marl

Hexyl alcohol (INCI)
Source : Henkel KGaA Duesseldorf

Hexyl alcohol, hexanol, C6 alcohol, hydroxyhexane, caproyl alcohol, pentylcarbinol, n-hexyl alcohol, amylcarbinol, 1-hydroxyhexane, amylcarbinol
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

Hexylalkohol
Source : Henkel KGaA Duesseldorf

n-Hexan-1-ol
Source : Henkel KGaA Duesseldorf

n-Hexanol
Source : Henkel KGaA Duesseldorf

N-Hexanol-1
Source : Henkel KGaA Duesseldorf

n-Hexyl alcohol
Source : Henkel KGaA Duesseldorf

Nansa EVM70/B
Source : Henkel KGaA Duesseldorf

Pentylcarbinol
Source : Henkel KGaA Duesseldorf

1.3 IMPURITIES

1.4 ADDITIVES

1.5 QUANTITY

Production during the last 12 months :

Import during the last 12 months	:	
Quantity	:	10 000 - 50 000 tonnes in

1.6.1 LABELLING

Labelling	:	as in Directive 67/548/EEC
Symbols	:	Xn
Nota	:	C
Specific limits	:	yes
R-Phrases	:	(22) Harmful if swallowed
S-Phrases	:	(2) Keep out of reach of children (24/25) Avoid contact with skin and eyes

1.6.2 CLASSIFICATION

Classification	:	as in Directive 67/548/EEC
Class of danger	:	corrosive
R-Phrases	:	(22) Harmful if swallowed

1.7 USE PATTERN

Type	:	type
Category	:	Non dispersive use
Type	:	type
Category	:	Wide dispersive use
Type	:	industrial
Category	:	Basic industry: basic chemicals
Type	:	industrial
Category	:	Chemical industry: used in synthesis
Type	:	industrial
Category	:	Personal and domestic use
Type	:	use
Category	:	Intermediates
Type	:	use
Category	:	Odour agents
Type	:	use
Category	:	Solvents

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit	:	MAK (DE)
Limit value	:	
Country	:	Germany
Remark	:	not established

Source : Huels AG Marl

(1)

1.9 SOURCE OF EXPOSURE

Remark : Industrial workers may be exposed during while handling.
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

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

Classified by : KBwS (DE)
Labelled by : KBwS (DE)
Class of danger : 1 (weakly water polluting)
Country : Germany
Remark : No. 125 in catalogue
Source : Huels AG Marl

(1)

Classified by : KBwS (DE)
Labelled by :
Class of danger : 1 (weakly water polluting)
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

1.14.2 MAJOR ACCIDENT HAZARDS

Legislation : Stoerfallverordnung (DE)
Substance listed : no
No. in directive :
Country : Germany
Remark : Stoerfallverordnung 1991
Source : Huels AG Marl

(1)

Legislation : Stoerfallverordnung (DE)
Substance listed : no
No. in directive :
Remark : Not a major accident hazard.

Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

1.14.3 AIR POLLUTION

Classified by	:	other: VCI
Labelled by	:	other: VCI
Number	:	3.1.7 (organic substances)
Class of danger	:	I
Country	:	Germany
Source	:	Huels AG Marl

(1)

1.15 ADDITIONAL REMARKS

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value	:	= -51.6 - ° C
Sublimation	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(2)

2.2 BOILING POINT

Value	:	= 157 - ° C at
Decomposition	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(3)

2.3 DENSITY

Type	:	density
Value	:	.81 - .82 g/cm3 at 20° C
Method	:	other: DIN 51757 B
Year	:	
GLP	:	no data
Test substance	:	
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(4)

Type	:	density
Value	:	.817 - .821 g/cm3 at 20° C
Method	:	other: DIN 51757
Year	:	
GLP	:	no
Test substance	:	
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(5)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	1 - hPa at 20° C
Decomposition	:	

Method		
Year	:	
GLP	:	no
Test substance	:	
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(5)

Value	:	ca. 2 - hPa at 40° C
Decomposition	:	
Method		
Year	:	
GLP	:	no data
Test substance	:	
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(4)

2.5 PARTITION COEFFICIENT

Log pow	:	= 1.95 - at ° C
Method		other (calculated): CLOGP program
Year	:	
GLP	:	no data
Test substance	:	
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(2)

2.6.1 WATER SOLUBILITY

Value	:	6 - g/l at 25 ° C
Qualitative	:	slightly soluble (0.1-100 mg/L)
Pka	:	at 25 ° C
PH	:	- at and ° C
Method	:	
Year	:	
GLP	:	no
Test substance	:	
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(5)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	62 ° C
Type	:	
Method	:	other: DIN 51755
Year	:	
GLP	:	no
Test substance	:	
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie

Hamburg

(5)

Value	:	ca. 65 ° C
Type	:	closed cup
Method	:	other: DIN 51758/ISO 2719 (According to Pensky-Martens)
Year	:	
GLP	:	no data
Test substance	:	
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(4)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

Result	:	non flammable
Method	:	Directive 84/449/EEC, A.13 "Flammability (solids and liquids)"
Year	:	
GLP	:	no
Test substance	:	
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

2.10 EXPLOSIVE PROPERTIES

Remark	:	No explosive properties.
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

2.11 OXIDIZING PROPERTIES

Remark	:	No oxidizing properties.
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

2.12 ADDITIONAL REMARKS

Remark	:	Solidification point: ca. -50 degr. C (according to DGF-C-IV-3c).
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(4)

3.1.1 PHOTODEGRADATION

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	other: mixture of soil and acclimated sludge from a domestic wastewater treatment plant.
Contact time	:	
Degradation	:	ca. 58.03 - % after 31 day
Result	:	other: These results indicate that the test substance is rapidly and extensively biodegraded
Deg. Product	:	
Method	:	other: modification of U.S. EPA TSCA method (40 CFR 796.3100)
Year	:	
GLP	:	no
Test substance	:	
Remark	:	From 20-24 mg of the test substance were added by weight to Teflon vial inserts which were then placed into their respective flasks. 30 ml of dichloromethane was then used to dissolve the test substance. The solvent was then evaporated leaving an film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(6)

Type	:	aerobic
Inoculum	:	other bacteria: municipal sewage treatment plant effluent
Concentration	:	2mg/l related to Test substance related to
Contact time	:	
Degradation	:	77 - % after 30 day
Result	:	readily biodegradable
Deg. Product	:	
Method	:	

Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Lorol C6
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(7)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	µg/l
Analytical monitoring	:	yes
LC50	:	97200 -
Method	:	other: not specified
Year	:	1983
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(8)

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	µg/l
Analytical monitoring	:	yes
LC50	:	97700 -
Method	:	other: not specified
Year	:	1984
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test substance	:	99% purity

(9)

Type	:	other: not specified
Species	:	Alburnus alburnus (Fish, estuary)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no data
LC50	:	= 120 -
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: see remarks
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test substance	:	The test substance was characterized as 98% pure 1-hexanol.

(10)

Type	:	static
Species	:	Alburnus albidus costa (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	µg/l
Analytical monitoring	:	no
LC50	:	120000 -
Method	:	other: not specified
Year	:	1979
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(11)

Type	:	static
Species	:	Alburnus alburnus (Fish, estuary)
Exposure period	:	96 hour(s)
Unit	:	µg/l
Analytical monitoring	:	no
LC50	:	120000 -
Method	:	other: not specified
Year	:	1984
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(12)

Type	:	static
Species	:	Brachydanio rerio (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	µg/l
Analytical monitoring	:	no
LC50	:	144000 -
Method	:	other: not specified
Year	:	1982
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(13)

Type	:	static
Species	:	Leuciscus idus (Fish, fresh water)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
LC0	:	30 -
LC50	:	55 -
LC100	:	100 -
Method	:	other: DIN 34412, part 15
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test substance	:	Lorol C6.

(7)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no data
EC50	:	201 -
Method	:	other: not specified
Year	:	1982
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie

Hamburg

(14)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC50	:	240 -
Method	:	other: not specified
Year	:	1977
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(15)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC0	:	152 -
Method	:	other: not specified
Year	:	1982
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(16)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	24 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC100	:	270 -
Method	:	other: not specified
Year	:	1982
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(17)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Anacystis aeruginosa (Algae)
Endpoint	:	growth rate
Exposure period	:	
Unit	:	µg/l
Analytical monitoring	:	no
LOEC	:	1200 -
Method	:	other: not specified
Year	:	1978
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(18)

Species	:	Anacystis aeruginosa (Algae)
Endpoint	:	other: lethality
Exposure period	:	
Unit	:	µg/l
Analytical monitoring	:	no data
LOEC	:	12000 -
Method	:	other: not specified
Year	:	1978
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(19)

Species	:	Euglena sp. (Algae)
Endpoint	:	growth rate
Exposure period	:	7 day
Unit	:	µg/l
Analytical monitoring	:	no data
LOEC	:	75000 -
Method	:	other: not specified
Year	:	1980
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(20)

Species	:	Scenedesmus quadricauda (Algae)
Endpoint	:	growth rate
Exposure period	:	7 day
Unit	:	µg/l
Analytical monitoring	:	no
LOEC	:	30000 -
Method	:	other: not specified
Year	:	1980
GLP	:	no data
Test substance	:	no data
Remark	:	This is the concentration in which a 3% in extinction value occurred.
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(20)

Species	:	Scenedesmus quadricauda (Algae)
Endpoint	:	growth rate
Exposure period	:	8 day
Unit	:	µg/l
Analytical monitoring	:	no
LOEC	:	30000 -
Method	:	other: not specified
Year	:	1978
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(21)

Species	:	Scenedesmus quadricauda (Algae)
Endpoint	:	growth rate
Exposure period	:	

Unit	:	µg/l
Analytical monitoring	:	no
EC50	:	30000 -
Method	:	other: not specified
Year	:	1977
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(22)

Species	:	other algae: Chilomonas paramecium
Endpoint	:	growth rate
Exposure period	:	48 hour(s)
Unit	:	µg/l
Analytical monitoring	:	no
LOEC	:	18000 -
Method	:	other: not specified
Year	:	1980
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(23)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type	:	aquatic
Species	:	Pseudomonas putida (Bacteria)
Exposure period	:	30 minute(s)
Unit	:	mg/l
Analytical monitoring	:	
EC0	:	1000 -
EC10	:	3000 -
Method	:	other: DIN 38412 Teil 8 (cell multiplication inhibition test)
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test substance	:	Lorol C6.

(7)

Type	:	aquatic
Species	:	Pseudomonas putida (Bacteria)
Exposure period	:	16 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC0	:	3000 -
EC10	:	10000 -
Method	:	other: DIN 38412 teil 27 (respiration inhibition test)
Year	:	
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test substance	:	Lorol C6.

(7)

Type	:	aquatic
Species	:	Tetrahymena pyriformis (Protozoa)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no data
EC50	:	300.4 -
Method	:	other: not specified
Year	:	1990
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(24)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

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

Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 4420 - mg/kg bw
Method	:	other: Not specified
Year	:	1977
GLP	:	no
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(25)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 3210 - mg/kg bw
Method	:	other
Year	:	
GLP	:	no
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(26)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 3131 - 3344 mg/kg bw
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(27)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 4900 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie

Hamburg

(28)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 4100 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(28)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 4870 - mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(29)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 4590 - mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(29)

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 4000 - mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA.

RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(29)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 103 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(2)

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 1950 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(2)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Exposure time	:	1 hour(s)
Value	:	> 21 - mg/l
Method	:	other
Year	:	1977
GLP	:	no
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(30)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	

Number of animals	:	
Vehicle	:	
Value	:	1500 - 2000 mg/kg bw
Method	:	other: not specified
Year	:	1977
GLP	:	no
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(31)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 2000 - mg/kg bw
Method	:	
Year	:	
GLP	:	no
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(32)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 2500 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(28)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	= 3100 - mg/kg bw
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(2)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	

Value	:	= 2530 - mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(29)

Type	:	LD50
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 5000 - mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(29)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type	:	LD50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	i.v.
Exposure time	:	
Value	:	= 100 - mg/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(29)

Type	:	other: lethality by aspiration
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Route of admin.	:	other: intratracheal
Exposure time	:	
Value	:	.2 - other: ml per animal
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	no data
Remark	:	Animals were induced to aspirate the test substance by

placing 0.2 ml of the test substance into the mouth and then closing the nostrils during inspiration. 10/10 animals died immediately. The cause of death was suspected to be respiratory or cardiac arrest, or both.

Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(33)

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : irritating
EC classification : irritating
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year :
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(34)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : moderately irritating
EC classification : irritating
Method : Draize Test
Year :
GLP : no
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(35)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : moderately irritating
EC classification : irritating
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year : 1984
GLP : yes
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(36)

Species : rabbit
Concentration :

Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	moderately irritating
EC classification	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(29)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	highly irritating
EC classification	:	irritating
Method	:	Draize Test
Year	:	
GLP	:	no
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(37)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	irritating
EC classification	:	irritating
Method	:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	:	1981
GLP	:	no data
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(34)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	moderately irritating
EC classification	:	irritating
Method	:	Draize Test
Year	:	
GLP	:	no

Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(38)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	moderately irritating
EC classification	:	irritating
Method	:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	:	1984
GLP	:	yes
Test substance	:	no data
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(39)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	highly irritating
EC classification	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(29)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	highly irritating
EC classification	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test substance	:	Hexanol, 98%.

(40)

5.3 SENSITIZATION

Type	:	Guinea pig maximization test
Species	:	guinea pig

Number of animals	:	
Vehicle	:	
Result	:	not sensitizing
Classification	:	
Method	:	other: Magnusson, B. Kligman, A.M. J. Invest. Dermatol., 52, 1969.
Year	:	1969
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(41)

Type	:	Guinea pig maximization test
Species	:	guinea pig
Number of animals	:	
Vehicle	:	
Result	:	not sensitizing
Classification	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(29)

Type	:	other: Human Maximization (as described by Epstein and Kligman)
Species	:	human
Number of animals	:	
Vehicle	:	
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	no data
Remark	:	The test substance was prepared and administered as a 1% solution of 1-hexanol in petrolatum.
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(42)

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male/female
Strain	:	no data
Route of admin.	:	oral feed
Exposure period	:	13 weeks
Frequency of treatment	:	food available ad lib, dietary mixture prepared weekly
Post obs. period	:	none
Doses	:	0%, 0.25%, 0.5% and 1% (2%,4%, 6% weeks 11,12,and 13, respectively)
Control group	:	yes
NOAEL	:	> .5 - %
LOAEL	:	= 1 - %
Method	:	other: See Remarks
Year	:	

GLP	:	no
Test substance	:	no data
Remark	:	Each test group consisted of ten males and ten females. The basal diet consisted of Purina Laboratory Chow. The compound was administered to the basal diet on a w/w basis and thoroughly mixed. Fresh diets were prepared each week. Body weights and food consumption were recorded weekly. Hematology studies and urine anlyses were conducted at 30 and 90 days. Organ and body weight measurements were made on all animals from each test group at the termination of the study (13 weeks). Selected tissues were obtained from each animal and preserved for possible microscopic examination. All of the selected tissues from the control and high dosage groups were examined microscopically.
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(43)

Species	:	dog
Sex	:	male/female
Strain	:	Beagle
Route of admin.	:	other: oral (dietary and capsule)
Exposure period	:	13 weeks
Frequency of treatment	:	test diet was available ad lib, the capsule was given six days per week (high dose group)
Post obs. period	:	none
Doses	:	0.5% (low), 1% (intermediate) and 1000 mg/kg (capsule, high dose)
Control group	:	other: basal diet only
NOAEL	:	= .5 - %
LOAEL	:	= 1 - %
Method	:	other: see remarks
Year	:	
GLP	:	no
Test substance	:	no data
Remark	:	The low and intermediate test groups consisted of two males and two females each. The high dose group (capsule) consisted of two males and three females. The basal diet consisted of ground Purina Dog meal. The compound was administered to the basal diet on a w/w basis and thoroughly mixed. Fresh diets were prepared each week. Body weights and feed consumption were recorded weekly. Hematological, plasma biochemistry, liver function and urine studies were performed on each dog during the pretreatment quarantine period, and at 3, 6, and 13 weeks. Organ and body weight measurements were made on all animals from each test group at the termination of the study (13 weeks). Selected tissues were obtained from each animal and preserved for possible microscopic examination. All of the selected tissues from the control and high dosage level animals were examined microscopically.
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(44)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella typhimurium
Concentration	:	8, 40, 200, 1000, and 5000 micrograms/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
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(45)

Type	:	Ames test
System of testing	:	Salmonella typhimurium
Concentration	:	6.25, 25, 100, 400, and 1600 micrograms/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
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(45)

5.6 GENETIC TOXICITY 'IN VITRO'

5.7 CARCINOGENITY

Species	:	mouse
Sex	:	no data
Strain	:	no data
Route of admin.	:	dermal
Exposure period	:	60 weeks
Frequency of treatment	:	three times a week for 60 weeks
Post. obs. period	:	none
Doses	:	20 microliters (20 grams of hexanol in 100 ml of cyclohexane)
Result	:	
Control group	:	no data specified
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	no data
Remark	:	The tumor-promoting activity of hexanol was studied on the skin of mice treated with an initiating dose of 7,12-dimethylbenz(a)anthracene, followed by the test substance. No skin tumours developed in 36 survivors.
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(42)

Species	:	mouse
Sex	:	

Strain	:	
Route of admin.	:	dermal
Exposure period	:	60 weeks
Frequency of treatment	:	3 times a week
Post. obs. period	:	
Doses	:	20 g in 100 ml cyclohexane
Result	:	
Control group	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	No tumors were observed.
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(29)

5.8 TOXICITY TO REPRODUCTION

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	days 1-19 of gestation
Frequency of treatment	:	7 hour/day
Duration of test	:	none
Doses	:	3500 mg/m3
Control group	:	yes
NOAEL Maternalt.	:	> 3500 -
NOAEL Teratogen	:	> 3500 -
Method	:	other: see remarks
Year	:	1989
GLP	:	no data
Test substance	:	other TS
Remark	:	Groups of approximately 15 sprague-dawley rats were exposed to 7 h/day on gestation days 1-19 to 3500 mg/m3 1-hexanol, which was the highest concentration which could be generated as a vapor. Dams were weighed daily for the first week of exposure and weekly thereafter and were sacrificed on day 20. Fetuses were serially removed, blotted dry, examined for external malformationa, sexed, weighed, fixed, and examined for visceral or skeletal defects.
Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Test substance	:	The purity of the test substance, which was described as reagent grade 1-hexanol, was >99% by gas chromatography using NIOSH analytical Method 1401.

(46)

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation

Exposure period	:	days 1-19 of gestation
Frequency of treatment	:	7 hours a day
Duration of test	:	
Doses	:	max. 3500 mg/m3
Control group	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	No signs of teratogenicity or embryotoxicity.
Source	:	Henkel KGaA. RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(29)

5.10 OTHER RELEVANT INFORMATION

5.11 EXPERIENCE WITH HUMAN EXPOSURE

6. References

(1) Huels AG: Sicherheitsdatenblatt "n-Hexanol", Version 04 (inaktiv), 07.10.1997

(2) Registry of Toxic Effects of Chemical Substances.

(3) Registry of Toxic Effects of Chemical Substances, online search 1995.

(4) MSDS Henkel KGaA. Lorol C 6 (DED 00003640 00, Ausgabe 01 vom 21.04.1994).

(5) Material Safety Data Sheets, NACOL 6M, NACOL 6-97, NACOL 6-98, NACOL-99, Condea Chemie GMbH, Version 1.00.02, Int. no. 0699003, 1994.

(6) Biodegradability of eleven VISTA ALFOL Alcohols. Technical Service Report, 6940-10-05-94, August 24, 1994.

(7) Henkel KGaA, unpublished data, Archive-No. 7198.

(8) Veith, G.D., et.al. Estimating the Acute Toxicity of Narcotic Industrial Chemicals to Fathead Minnows. In: W.E. Bishop, R.D. Cardwell, and B.B. Heidolph (Eds.), Aquatic Toxicology and Assessment, 6th symposium, ASTM STP 802, Philadelphia, PA:90-97, 1983.

(9) Brooke, L.T., et.al. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, Vol.1, WI:414, 1984.

(10) Merck, E.G. undated.

(11) Linden, E. The Acute Toxicity of 78 Chemicals and Pesticide Formulationa Against Two Brackish Water Organisms, The Bleak (Alburnus alburnus) and the Harpacticoid Ni,. Chemosphere, Vol. 8, No. 11/12, pgs. 843-851, 1979.

(12) Bengtsson, B.E., et. al. Molecular Structure and Aquatic Toxicity- An Example with C1-C13 Aliphatic Alcohols. Chemosphere, Vol. 13, No. 5-6, Pgs. 613-622, 1984.

(13) Wellens, H. Comparison of the Sensitivity of Brachydanio rerio and Leuciscus idus by Testing the Fish Tosicity of Chemicals and Wastewaters. Z. Wasser Abwasser Forsch. Vol.15, No. 2, Pgs. 49-52, 1982.

(14) Brigham, G. and Kuhn, R. The Results of Toxic Action of Water Pollutants on Daphnia magna Straus Tested by an Improved Standardized Procedure. Z. Wasser Abwasser Forsch., Vol. 15, No. 1, Pgs. 1-6, 1978.

(15) Bringham, G. and Kuhn, G. Results of the Damaging Effect of Water Pollutants on Daphnia Magna. Z. Wasser Abwasser Forsch., Vol. 10, No. 5, pgs. 161-166, 1977.

(16) Brigham, G. and Kuhn, R. Results of Toxic Action of Water Pollutants on Daphnia magna Straus Tested by an Improved Standardized procedure. Z. Wasser Abwasser Forsch., Vol. 15, No. 1, Pgs. 1-6, 1982.

(17) Bringham, G. and Kuhn, R. Results of Toxic Action of Water Pollutants on Daphnia magna Straus Tested by an improved Standardized Procedure. Z. Wasser Abwasser Forsch., Vol. 15, No. 1, Pgs. 106, 1982.

(18) Brigham, G. and Kuhn, R. Testing of Substances for Their Toxicity Threshold: Model Organisms Microcystis (Diplocystis) aeruginosa and Scendesmus quadricauda. Mitt. Int. Ver. Theor. Angew. Limnol, Vol. 21, Pgs. 275-284, 1978.

(19) Bringham, G. and Kuhn, G. Limiting Values for the Noxious Effects of Water Pollutants to Blue Algae (Microcystis aeruginosa and Green Algae (Scendesmus quadricauda) in the . . . Z. Vom. Wasser., Vol. 50, pgs. 45-60, 1978.

(20) Bringham, G. and Kuhn, G. Comparison of the Toxicity Threshold of Water Pollutants to Bacteria, Algae, and Protozoa in the Cell Multiplication Inhibition Test. Water Res., Vol. 14, No. 3, pgs. 231-241, 1980.

(21) Brigham, G. and Kuhn, R. Testing of Substances for Their Toxicity Threshold: Model Organisms Microcystis (Diplocystis) aeruginosa and Scendesmus quadricauda. Mitt. Int. Ver. Theor. Angew. Limnol, Vol. 21, Pgs. 275-784, 1978.

(22) Bringham, G. and Kuhn,G. Limiting Values for the Damaging Action of Water Pollutants to Bacteria (Pseudomonas putida) and Green Algae (Scendesmus quadricauda) in the . . . Z. Wasser Abwasser Forsch., Vol. 10, No. 3/4, pgs. 87-98, 1977.

(23) Brigham, G. and Kuhn, R. Determination of Biological Damage From Water Pollutants to Protozoa. III. Saprozoic Flagellates.
Z. Wasser Abwasser Forsch., Vol. 13, No. 5, Pgs. 170-173, 1980.

(24) Schultz, T.W., et. al. Relationships of Quantitative Structure-Activity for Normal Aliphatic Alcohols. Ecotoxicol. Environ. Saf., Vol. 19, No. 3, pgs. 243-253, 1990

(25) Acute Oral Toxicity (LD50) in Rats, ALFOL 6 Alcohol, Scientific Associates, Inc. for Continental Oil Company, November 23, 1977.

(26) Acute Oral Toxicity (LD50) in Rats, ALFOL 6 Alcohol, Scientific Associates, Inc. for Continental Oil Company, April 29, 1965.

(27) Acute Oral Toxicity in Rats, NACOL 6 RD, Laboratory of Pharmacology and Toxicology, for Condea Chemie GmbH, February 11, 1987.

(28) Dangerous Properties of Industrial Materials Report. Hexanol. Nov/Dec, 1987.

(29) Primaerliteratur cited in: Henkel KGaA, unpublished data, Archive-No. TBD 910457.

(30) Acute Inhalation Toxicity (LC50) in Rats, ALFOL 6 Alcohol, Scientific Associates, Inc. for Continental Oil Company, April 29, 1965.

(31) Acute Dermal Toxicity (LD50) in Rabbits. Scientific Associates, Inc. for Continental Oil Company, November 23, 1977.

(32) Acute Dermal Toxicity (LD50) in Rabbits. Alfol 6 alcohol. Scientific Associates, Inc. for Conco, Inc., November 28, 1980.

(33) Gerare, H. and Ahlstrom, D. The Aspiration Hazard and Toxicity of a Homologous Series of Alcohols. Arch. Environ. Health, Vol. 13, October, 1966.

(34) Guido, J. and Martens, Mark, A. Skin and Eye Irritation Tests on Hexanol. J. AM. Coll. Toxicol. Vol. 11, No. 6, pg. 722, 1987.

(35) Acute Dermal Toxicity (LD50) in Rabbits, ALFOL 6 Alcohol, Scientific Associates, Inc. for Continental Oil Company, April 29, 1965.

(36) Acute Skin Irritation/Corrosion Test (Patch-Test) Of NACOL 6 RD in The RAbbit. Condea Chemie GmbH, November 17, 1986.

(37) Acute Eye Irritation in Rabbits, ALFOL 6 Alcohol, Scientific Associates, Inc. for Continental Oil Company, April 29, 1965.

(38) Primary Eye Irritation in Rabbits, ALFOL 6 Alcohol, Hazleton Raltech, Inc. ciates, Inc. for Conco, Inc., December 4, 1982.

(39) Eye Irritation Study of NACOL 6 RD in the Rabbit After single Instillation into the Conjunctival Sac. Laboratory of Pharmacology and Toxicology for Condea Chemie GmbH, November 18, 1986.

(40) ECETOC, Eye Irritation: Reference Chemicals Data Bank, Technical Report No. 48, 1992.

(41) Henkel KGaA, unpublished data, Archive-no. TBD 790129.

(42) Patty's Industrial Hygiene and Toxicology. V.K. Rowe and S.B. McCollister, Third Revised Edition, pg.4610.

(43) Final Report- Thirteen-Week Sub Acute Feeding of ALFOL 6 to rats, Scientific Associates for Continental Oil Company, April, 1966.

(44) Final Report On Thirteen-Week Subacute Feeding In Beagle Dogs of ALFOL 6, Scientific Associates for Continental Oil Company,
June 14, 1966.

(45) Henkel KGaA, Unpublished data, Archive-No. TBD 900320.

(46) Nelson, B.K., et.al. Developmental Toxicology Evaluation of 1-Pentanol, 1-hexanol, and 2-Ethyl-1-Hexanol Administered by Inhalation to Rats. J. Amer. Coll. Tox., Vol. 8, No. 2,
Pgs. 405-410, 1989.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT