IUCLID

Data Set

Existing Chemical	:	ID: 598-98-1
CAS No.	:	598-98-1
EINECS Name	:	methyl pivalate
EC No.	:	209-959-1
TSCA Name	:	Propanoic acid, 2,2-dimethyl-, methyl ester
Molecular Formula	:	C6H12O2

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001
Status	:	
Memo	:	ExxonMobil Chemical Company (EMCC) Neoacids - HPV
Printing date	:	06.11.2006
Revision date	:	
Date of last update	:	16.10.2006
Number of pages	:	23
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Neoacids C5 to C28 Category is a group of Neoacids whose physicochemical and toxicological properties are very similar and follow a regular pattern as a result of synthesis and structural similarity. The production of neoacid products involves the reaction between a branched olefin with carbon monoxide and water at elevated temperatures and pressures in the presence of an acid catalyst. The products in this category range in carbon number from C5 to C28.

The six substances share relatively similar physico-chemical properties, which suggests that their environmental fate will be similar. Neoacids are trialkylacetic acids in which each hydrogen on the non carboxyl carbon of acetic acid has been replaced by an alkyl group. There is also a likelihood of common precursors and breakdown products that can result in structurally similar metabolites (e.g. carboxylic acid). Because these substances are similar with regard to environmental behavior/effects and human health, consideration of these substances as a category is justified.

The category also contains propanoic acid, 2,2-dimethyl-, methyl ester (CAS#: 598-98-1). This material is an ester that is rapidly hydrolyzed to the parent neoacid - propanoic acid, 2,2-dimethyl- (CAS#: 75-98-9). Because of this rapid hydrolysis, propanoic acid, 2,2-dimethyl-, methyl ester has properties for health effects, aquatic toxicity, and environmental fate that are consistent with the neoacids.

01.09.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C6H12O2
Molecular weight : 116.16
Petrol class :

Flag : Critical study for SIDS endpoint
21.09.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid

Purity :
Colour :
Odour :

Remark : CAS Registry Number, Name, and General Structure for Members of the Neoacids C5 to C28 Category and Analogue Substances:

CAS RN: 598-98-1
IUPAC Name: methyl pivalate
R length (C number): C6
Structure of R: Linear
Category Member: Yes

21.09.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

methyl pivalate

11.11.2004

1.3 IMPURITIES

Purity : typical for marketed substance
CAS-No : 598-98-1
EC-No : 209-959-1
EINECS-Name : methyl pivalate
Molecular formula : C6H12O2
Value : = 99 % w/w

21.09.2006

1.4 ADDITIVES

Purity type : typical for marketed substance
CAS-No :
EC-No :
EINECS-Name :
Molecular formula :
Value :
Function of additive :

Remark : No additives present.
21.09.2006

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Chemical industry: used in synthesis

Remark : Primarily used as a component in the production of vinyl chloride resins.
21.09.2006

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -62.5 °C
Sublimation	:	
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Test substance	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

21.09.2006 (3)

2.2 BOILING POINT

Value	:	= 101 °C at 1013 hPa
Decomposition	:	
Method	:	other: D1078/01
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

16.10.2006 (4)

2.3 DENSITY

Type	:	density
Value	:	= .87 g/cm³ at 20 °C
Method	:	other: ASTM D4052/86 equivalent
Year	:	2003
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

21.09.2006 (4)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 47.6 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential vapor pressure for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

21.09.2006 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 1.8 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Remark	:	Value was provided by the experimental database of the EPIWIN program.
Test substance	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

21.09.2006 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 2835 mg/l at 25 °C
pH value	:	

concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	4.6 at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	

Method	:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential water solubility for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

21.09.2006 (3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 7 °C
Type	:	closed cup
Method	:	other: TCC ASTM D56
Year	:	2003
GLP	:	
Test substance	:	

Test substance	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

21.09.2006 (4)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	4.6
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux Calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on the chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

21.09.2006 (5)

2.13 VISCOSITY

Value	:	= 1 - at 25 °C
Result	:	
Method	:	other: ASTM D445
Year	:	2003
GLP	:	no data
Test substance	:	
Remark	:	Value measured in cSt
Test substance	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.

21.09.2006 (4)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000007194 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year	:	2003
GLP	:	
Test substance	:	

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (days)	OH- Rate Constant (cm3/molecule-sec)
14.9	0.7194 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C

Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester

Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.

Flag : Critical study for SIDS endpoint
21.09.2006 (3)

Type : water
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
Deg. product :
Method : other (calculated): Technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterizing the potential of substances in the Neoacids C5 to C28 Category to undergo direct photodegradation.

Result : Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Neoacids C5 to C28 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References:

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Boethling, R.S., Mackay, D. 2000. Handbook of Property Estimation Methods for Chemicals, CRC Press, Boca Raton, FL, USA.

Test substance : Neoacids C5 to C28 Category members
Flag : Critical study for SIDS endpoint
01.09.2006 (2)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method : other: technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterising the potential of substances in the Neoacids C5 to C28 Category to undergo hydrolysis.
Result : Hydrolysis as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

Chemicals that are susecptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances 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). The lack of a suitable leaving group renders a compound resistant to hydrolysis.

Aliphatic acids are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982).

References:

Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

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.

Test substance : Neoacids C5 to C28 Category members
Conclusion : Hydrolysis will not contribute to the removal of neoacids from the environment.

Flag : Critical study for SIDS endpoint
01.09.2006 (1)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 116.16 g/mol
Water solubility = 2835 mg/L
Vapour pressure = 4760 Pa
log Kow = 1.8
Melting point = -62.5 deg C

Degradation half-lives:

Air - 178 hrs
Water - 2400 hrs
Soil - 72000 hrs
Sediment - 720000 hrs

This model was run assuming 100% discharge to water.

Result :

Air - 13.7%
Water - 86.0%
Soil - 0.03%
Sediment - 0.28%

Test substance : CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester

Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
21.09.2006		(6)

Type	:	fugacity model level I
Media	:	other: air - biota - sediment(s) - soil - water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation according Mackay, Level I
Year	:	2003

Method :

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.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:

Molecular mass = 116.16 g/mol
Water solubility = 2835 mg/L
Vapour pressure = 4760 Pa
log Kow = 1.8
Melting point = -62.5 deg C

Result :

Soil - 0.1%
Air - 97.1%
Water - 2.5%
Sediment - <0.01%
Suspended Sed - <0.01%
Biota - <0.01%

Test substance	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester
Conclusion	:	Results of the Mackay Level I environmental distribution model suggest that Neoacids C5 to C28 Category substances have a potential to partition to soil and air. However, category members are weak organic acids with estimated dissociation constants (pKa) of 4.6 to 4.9 (Karickoff, et. al. 1991). Consequently, category substances at neutral pH, which is typical of most natural surface waters, are expected to dissociate (>99%) to the ionized form and therefore, remain largely in water. The Mackay model is usually limited to non-ionic organics and according to Harris and Hayes, 1982, the ionized species of organic acids are generally adsorbed by soils and sediments to a much lesser degree than are the neutral forms. As a result the Mackay model may overestimate the partitioning of Neoacids C5 to C28 Category substances to the soil and sediment compartments.
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
21.09.2006		(6)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF	:	= 5.12 -
Elimination	:	
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Calculated values using BCFWIN version 2.13, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	BCFWIN estimates the bioconcentration factor (BCF) of an organic compound using the compound's log octanol-water partition coefficient (Kow). The estimation methodology used by BCFWIN is described in "Improved Method for Estimating Bioconcentration Factor (BCF) from Octanol-Water Partition Coefficient", SRC TR-97-006 (2nd Update), July 22, 1997. Log Kow used = 1.83
Test substance	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential bioaccumulation factor for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

22.09.2006 (3)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) EMBSI (2005) Hydrolysis: Neoacids C5 to C28 Category.

(2) EMBSI (2005) Photodegradation (Direct): Neoacids C5 to C28 Category.

(3) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(4) ExxonMobil Chemical Company (2003). Methyl Pivalate. Unpublished internal data.

(5) Karickoff, S.W., V.K. McDaniel, C. Melton, A.N. Vellino, D.E. Nute, L.A. Carreira (1991). Predicting chemical reactivity by computer. Environ. Toxicol. Chem. 10:1405-1416.

(6) Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model ver. 2.02, available from the Environmental Centre, Trent University, Canada.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 75-98-9
CAS No.	:	75-98-9
EINECS Name	:	pivalic acid
EC No.	:	200-922-5
TSCA Name	:	Propanoic acid, 2,2-dimethyl-
IUPAC Name	:	pivalic acid
Molecular Formula	:	C5H10O2

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001
Status	:	
Memo	:	ExxonMobil Chemical Company (EMCC) Neo Acids - HPV
Printing date	:	06.11.2006
Revision date	:	
Date of last update	:	16.10.2006
Number of pages	:	35
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Neoacids C5 to C28 Category is a group of Neoacids whose physicochemical and toxicological properties are very similar and follow a regular pattern as a result of synthesis and structural similarity. The production of neoacid products involves the reaction between a branched olefin with carbon monoxide and water at elevated temperatures and pressures in the presence of an acid catalyst. The products in this category range in carbon number from C5 to C28.

The six substances share relatively similar physico-chemical properties, which suggests that their environmental fate will be similar. Neoacids are trialkylacetic acids in which each hydrogen on the non carboxyl carbon of acetic acid has been replaced by an alkyl group. There is also a likelihood of common precursors and breakdown products that can result in structurally similar metabolites (e.g. carboxylic acid). Because these substances are similar with regard to environmental behavior/effects and human health, consideration of these substances as a category is justified.

The category also contains propanoic acid, 2,2-dimethyl-, methyl ester (CAS#: 598-98-1). This material is an ester that is rapidly hydrolyzed to the parent neoacid - propanoic acid, 2,2-dimethyl- (CAS#: 75-98-9). Because of this rapid hydrolysis, propanoic acid, 2,2-dimethyl-, methyl ester has properties for health effects, aquatic toxicity, and environmental fate that are consistent with the neoacids.

01.09.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C5H10O2
Molecular weight : 102.13
Petrol class :

Flag : Critical study for SIDS endpoint
01.09.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid

Purity :
Colour :
Odour :

Remark : CAS Registry Number, Name, and General Structure for Members of the Neoacids C5 to C28 Category and Analogue Substances:

CAS RN: 75-98-9
IUPAC Name: pivalic acid
R length (C number): C5
Structure of R: Linear
Category Member: Yes

01.09.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

neopentanoic acid

10.11.2004

Pivalic acid

10.11.2004

Propanoic acid, 2,2-dimethyl-

19.11.2001

trimethyl acetic acid

10.11.2004

1.3 IMPURITIES

Purity : typical for marketed substance
CAS-No : 75-98-9
EC-No : 200-922-5
EINECS-Name : pivalic acid
Molecular formula : C5H10O2
Value : = 99.7 % w/w

01.09.2006

1.4 ADDITIVES

Purity type : typical for marketed substance
CAS-No : 75-98-9
EC-No : 200-922-5
EINECS-Name : pivalic acid
Molecular formula :
Value :
Function of additive :

Remark : No additives present
01.09.2006

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Chemical industry: used in synthesis

Remark : Primarily used as a chemical intermediate in the production of synthetic lubricants or hydraulic fluids.

01.09.2006

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 35 °C
Sublimation	:	
Method	:	other: calculated
Year	:	2003
GLP	:	no
Test substance	:	
Method	:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

01.09.2006 (16)

2.2 BOILING POINT

Value	:	= 163 - 165 °C at 1013 hPa
Decomposition	:	
Method	:	other: D1078/01
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

01.09.2006 (9)

2.3 DENSITY

Type	:	density
Value	:	= .91 g/cm³ at 20 °C
Method	:	other: ASTM D4052/86 equivalent
Year	:	2003
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

01.09.2006 (9)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 2.05 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential vapor pressure for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

01.09.2006 (14)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 1.5 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Remark	:	Value was provided by the experimental database of the EPIWIN program.
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

01.09.2006 (17)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 15590 mg/l at 25 °C
pH value	:	

concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	4.6 at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	

Method	:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential water solubility for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

15.09.2006 (16)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 62.8 °C
Type	:	closed cup
Method	:	other: TCC ASTM D56
Year	:	2003
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

15.09.2006 (9)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	4.6
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux Calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability	:	(2) valid with restrictions The value was calculated based on the chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

15.09.2006 (11)

2.13 VISCOSITY

Value	:	= 3.6 - at 60 °C
Result	:	
Method	:	other: ASTM D445
Year	:	2003
GLP	:	no data
Test substance	:	
Remark	:	Value measured in cSt
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.

15.09.2006 (9)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000010218 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year	:	2003
GLP	:	
Test substance	:	

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (days)	OH- Rate Constant (cm3/molecule-sec)
10.5	1.0218 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C

Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-

Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.

Flag : Critical study for SIDS endpoint
15.09.2006 (15)

Type : water
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
Deg. product :
Method : other (calculated): Technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterizing the potential of substances in the Neoacids C5 to C28 Category to undergo direct photodegradation.

Result : Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Neoacids C5 to C28 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References:

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Boethling, R.S., Mackay, D. 2000. Handbook of Property Estimation Methods for Chemicals, CRC Press, Boca Raton, FL, USA.

Test substance : Neoacids C5 to C28 Category members
Flag : Critical study for SIDS endpoint
01.09.2006 (4)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method : other: technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterising the potential of substances in the Neoacids C5 to C28 Category to undergo hydrolysis.
Result : Hydrolysis as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

Chemicals that are susecptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances 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). The lack of a suitable leaving group renders a compound resistant to hydrolysis.

Aliphatic acids are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982).

References:

Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

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.

Test substance : Neoacids C5 to C28 Category members
Conclusion : Hydrolysis will not contribute to the removal of neoacids from the environment.

Flag : Critical study for SIDS endpoint
01.09.2006 (3)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 102.13 g/mol
Water solubility = 15590 mg/L
Vapour pressure = 205 Pa
log Kow = 1.5
Melting point = 35 deg C

Degradation half-lives:

Air - 126 hrs
Water - 2400 hrs
Soil - 72000 hrs
Sediment - 720000 hrs

This model was run assuming 100% discharge to water.

Result :

Air - 0.78%
Water - 98.7%
Soil - 0.27%
Sediment - 0.26%

Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-

Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
18.09.2006		(13)
Type	:	fugacity model level I
Media	:	other: air - biota - sediment(s) - soil - water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation according Mackay, Level I
Year	:	2003
Method	:	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. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). Input values used: Molecular mass = 102.13 g/mol Water solubility = 15590 mg/L Vapour pressure = 205 Pa log Kow = 1.5 Melting point = 35 deg C
Result	:	Soil - 0.1% Air - 97.4% Water - 2.5% Sediment - <0.01% Suspended Sed - <0.01% Biota - <0.01%
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion	:	Results of the Mackay Level I environmental distribution model suggest that Neoacids C5 to C28 Category substances have a potential to partition to soil and air. However, category members are weak organic acids with estimated dissociation constants (pKa) of 4.6 to 4.9 (Karickoff, et. al. 1991). Consequently, category substances at neutral pH, which is typical of most natural surface waters, are expected to dissociate (>99%) to the ionized form and therefore, remain largely in water. The Mackay model is usually limited to non-ionic organics and according to Harris and Hayes, 1982, the ionized species of organic acids are generally adsorbed by soils and sediments to a much lesser degree than are the neutral forms. As a result the Mackay model may overestimate the partitioning of Neoacids C5 to C28 Category substances to the soil and sediment compartments.
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
18.09.2006		(12)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge, domestic
Contact time	:	28 day(s)
Degradation	:	= 24 (±) % after 28 day(s)
Result	:	inherently biodegradable
Deg. product	:	
Method	:	OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year	:	1996
GLP	:	yes
Test substance	:	
Remark	:	Test Type: Manometric Respirometry Test
Result	:	Test material was not readily biodegradable. Half-life was not reached. By day 28, 24% degradation of the test material was observed. 10% biodegradation was achieved on day 20 By day 14, >60% biodegradation of positive control was observed, which meets 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	18.9, 42.7, 10.7	24.1
Na Benzoate	98.9, 95.5	97.2

* replicate data

Test condition	:	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 between 31 and 50 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.
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion	:	Test substance is considered not readily biodegradable.
Reliability	:	(1) valid without restriction

18.09.2006 (7)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF	:	= 3.16
Elimination	:	
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Calculated values using BCFWIN version 2.13, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	BCFWIN estimates the bioconcentration factor (BCF) of an organic compound using the compound's log octanol-water partition coefficient (Kow). The estimation methodology used by BCFWIN is described in "Improved Method for Estimating Bioconcentration Factor (BCF) from Octanol-Water Partition Coefficient", SRC TR-97-006 (2nd Update), July 22, 1997. Log Kow used = 1.48
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential bioaccumulation factor for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

22.09.2006 (5)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Carassius auratus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Limit test	:	no
Analytical monitoring	:	yes
Method	:	other: Standard Methods for the Examination of Water and Wastewater Method #231, 1971
Year	:	1979
GLP	:	no
Test substance	:	
Remark	:	Statistical Method: Interpolation of graph of log of concentration (APHA 1971).
Result	:	LC50 = 380mg/L Analytical method used was Total Organic Carbon or by extraction and subsequent GC analysis.
Test condition	:	The test material was added to ~30 L glass tank containing laboratory dilution water. Each chemical was tested in a series of concentrations in 25 L of solution. All tanks contained 10 fish. All test solutions were aerated unless it was a volatile compound. Test temperature was 20 +/- 1 Deg C., Lighting was not reported Dissolved Oxygen = test solutions aerated during study. The pH was 5.4. Fish Mean Wt.= 3.3 +/- 1.0g. Mean Total length = 6.2 +/-cm, Test Loading = 1.3 g of fish/L.
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion	:	Test substance is considered to have low toxicity.
Reliability	:	(2) valid with restrictions Minimal data presented (i.e. lacking conc. series, analytical measurements, Dissolved Oxygen measurements).
Flag	:	Critical study for SIDS endpoint

18.09.2006 (1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Limit Test	:	no
Analytical monitoring	:	no
Method	:	other: USEPA -660/3-75-009 Methods for Acute Toxicity with Fish and Macroinvertebrates, and Amphibians, 1975
Year	:	1977
GLP	:	no data
Test substance	:	
Remark	:	Daphnid Acute Toxicity Test Statistical Method: Moving Average-Angle Method, (Harris 1959)
Result	:	LC50 = 202.94 mg/L (95% CI 241.23 to 168.21) based upon nominal test concentrations. Mean % Mortality

Test Concentration	24 hr.	48 hr.
Positive Control	0	0
Negative Control	0	0
36 mg/L	0	0
60 mg/L	0	0
100 mg/L	0	7
170 mg/L	7	13
280 mg/L	20	93
460 mg/L	100	100

Test condition : For each test concentration, the appropriate amount of test substance was dissolved in ethanol and pipetted into 500ml of dilution water. This solution was mixed with a magnetic stirrer and divided into three 150ml replicates for testing. The remaining 50ml was used for pH and dissolved oxygen measurements. A positive control (with ethanol) and a negative control (dilution water) were also tested. Test vessels were 250ml beakers containing five daphnids each. Dilution water was reconstituted deionized water with a hardness of 180mg/L as CaCO3, with a pH of 8.0. The test was performed under static conditions with no aeration.

Nominal test concentrations were 36, 60, 100, 170, 280, and 460 mg/L

Test temperature was 22+/- 1 Deg C. Dissolved oxygen ranged from 8.6 to 8.8 mg/L during the study. The pH of the test solutions varied from Control - 8.3; 36 mg/L - 8.2; 170 mg/L - 7.6; and 460 mg/L - 5.2.
Organisms were supplied by in-house cultures. Age = <24 hours old

Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-

Conclusion : Test substance is considered to be of low toxicity.

Reliability : (2) valid with restrictions
Lack of analytical verification, concentration of ethanol unknown, missing pH value of 280mg/L concentration, quality assurance unknown.

Flag : Critical study for SIDS endpoint

18.09.2006 (2)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae: Pseudokirchneriella subcapitata

Endpoint : biomass

Exposure period : 72 hour(s)

Unit : mg/l

NOEC : = 246 measured/nominal

EC50 : = 878 measured/nominal

Limit test : no

Analytical monitoring : yes

Method : OECD Guide-line 201 "Algae, Growth Inhibition Test"

Year : 2003

GLP : yes

Test substance :

Remark : Statistical Procedure - Proc regression procedure of SAS, Anova procedure of SAS for NOEC

Result : 72 hour EC50b=878 mg/L (biomass)
72 hour EC50gr=979 mg/L (growth rate)

72 hour NOECb=246 mg/L (biomass)
72 hour NOECgr=246 mg/L (growth rate)

Nominal	Mean Cell Biomass - 72 hr	Mean Cell Conc. - 72 hr

Conc. (mg/L)	(% Inhibition)	(cells/ml)
Control	n/a	7.0 x105
62	1.5	6.9 x105
125	-3.0	7.2 x105
250	-1.0	7.1 x105
500	24	5.3 x105
1000	64	2.4 x105

n/a - Not applicable
note: a negative value indicates a stimulatory effect.

Test condition : Individual test treatment solutions were prepared as Water Accommodated Fractions (WAFs). Test material was added to algal media in 2.0L aspirator bottles. The vessels were mixed on magnetic stir plates with teflon coated stir bars for 23 hours at room temperature. After mixing the solutions were allowed to settle for one hour and the aqueous portion of the WAF was removed from the bottom of the mixing vessel via the port and used for testing. Test vessels were 125ml glass Erlenmeyer flasks with approximately 60 ml of treatment solution and inoculated with algae. Test vessels were sealed with foam stoppers. Samples were taken daily for cell counts. Four replicates were prepared for each treatment level. The initial algal concentration was 1.0 x 104 cells/ml. All test replicates were placed on a shaker table at 100 oscillations per minute during the study. Biomass was calculated as the area under the growth curve.

Nominal loading levels were 62, 125, 250, 500, and 1000 mg/L

Test treatments were analyzed by GC-FID on Day 0 and at termination. Mean measured values were 54.8, 128, 246, 488 and 979 mg/L. The test material was not detected in the control.

Test temperature was 23.4 Deg. C. Lighting was continuous at 7229 to 7586 Lux. The pH was 7.4 to 7.6 at test initiation and ranged from 7.1 to 7.5 at test termination.

Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
18.09.2006 (8)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 2000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	5
Vehicle	:	other: none
Doses	:	
Method	:	other
Year	:	1964
GLP	:	no
Test substance	:	
Remark	:	Route of administration: Gastric Intubation Frequency of Treatment: Single Dose Dose/Concentration Levels: 34.6, 120, 417, 1450, 5000, and 10000 mg/kg Control group and Treatment: None There were no deaths and no findings at necropsy in animals treated with 34.6, 120 and 417 mg/kg. At the 1450 mg/kg level, 2 of 5 animals died by day 2 and the remaining animals survived until the end of the study. These animals showed depression, severe dyspnea, depressed reflexes, sprawling, and lack of coordination. All animals in the 5000 and 10,000 mg/kg dose groups died within 48 hours of treatment. Severe depression, dyspnea, and prostration preceded death in all of the animals that died. Necropsy findings in high dose animals indicated congestion of lungs, liver, kidneys, and adrenals.
Result	:	LD50= 2000 mg/kg (CL: 830 to 4820 mg/kg) Number of animals dead per number tested: 34.6, 120 and 417 mg/kg: 0/5 1450 mg/kg: 2/5 5000 mg/kg: 5/5 10,000 mg/kg: 5/5
Test condition	:	The animals were fasted for a period of three to four hours prior to treatment. The animals were observed for toxic effects and mortality at one, four and 24 hours; and once daily thereafter for 14 days. A necropsy was performed on any animal that died. All surviving animals were weighed, sacrificed and necropsied.
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion	:	Under conditions of this study, Propanoic acid, 2,2-dimethyl- acid has a low order of acute oral toxicity in rats.
Reliability	:	(2) valid with restrictions Study was performed Pre-GLP
Flag	:	Critical study for SIDS endpoint

18.09.2006 (6)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 4 mg/l
Species	:	rat
Strain	:	Wistar

Sex	:	male
Number of animals	:	10
Vehicle	:	
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1964
GLP	:	no
Test substance	:	

Remark : No deaths occurred among any of the animals during the inhalation exposure. Two rats died on the second and fifth days. Rats displayed piloerection, epitasis, and dyspnea following exposure. Due to advanced autolysis, necropsy of the animals that died did not reveal any meaningful findings. Necropsy of the animals that survived until termination of the study did not reveal any significant gross pathology.

Route of administration: Inhalation
Frequency of Treatment: Single 6-hour exposure
Dose/Concentration Levels: Saturated vapors - the mean nominal concentration was 4.0 mg/L.

Control group and Treatment: A group of rats that served as a common control for the substances tested in this study were sacrificed and examined grossly.

Result : Rat > 4.0 mg/L

Test condition : An atmosphere of saturated vapors was produced by forcing air through a bubbler system that contained the test substance. 29 ml of liquid was vaporized at a flow rate of 23 L/min. Animals were caged in wire mesh compartments within the exposure chamber. Animals were observed for mortality and toxic effects at 30-minute intervals during exposure and daily thereafter. The animals were observed for two weeks following exposure, at which point animals were sacrificed and necropsied. Any animals that died during the exposure or observation periods were necropsied.

Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-

Conclusion : Propanoic acid, 2,2-dimethyl- has a moderate order of inhalation toxicity in rodents.

Reliability : (2) valid with restrictions
No vapor concentration verification (analytical). Study was performed pre-GLP regulations.

Flag : Critical study for SIDS endpoint

18.09.2006 (6)

Type	:	LC50
Value	:	< 4 mg/l
Species	:	mouse
Strain	:	other: Swiss albino
Sex	:	male
Number of animals	:	10
Vehicle	:	
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1964
GLP	:	no
Test substance	:	

Remark : No deaths occurred among any of the animals during the inhalation exposure. Hyperactivity followed by prostration was observed in mice. All 10 mice died within the 24 hours following exposure. Due to advanced autolysis, necropsy of the animals that died did not reveal any meaningful findings. Necropsy of the animals that survived until termination of the

study did not reveal any significant gross pathology.

Route of administration: Inhalation
Frequency of Treatment: Single 6-hour exposure
Dose/Concentration Levels: Saturated vapors - the mean nominal concentration was 4.0 mg/L.

Control group and Treatment: A group of mice that served as a common control for the substances tested in this study were sacrificed and examined grossly.

Result : Mouse LC50 < 4.0 mg/L
Test condition : An atmosphere of saturated vapors was produced by forcing air through a bubbler system that contained the test substance. 29 ml of liquid was vaporized at a flow rate of 23 L/min. Animals were caged in wire mesh compartments within the exposure chamber. Animals were observed for mortality and toxic effects at 30-minute intervals during exposure and daily thereafter. The animals were observed for two weeks following exposure, at which point animals were sacrificed and necropsied. Any animals that died during the exposure or observation periods were necropsied.
Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion : Propanoic acid, 2,2-dimethyl- has a moderate order of inhalation toxicity in rodents.
Reliability : (2) valid with restrictions
No vapor concentration verification (analytical). Study was perfomed pre-GLP.
Flag : Critical study for SIDS endpoint
18.09.2006 (6)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : = 3160 mg/kg bw
Species : rabbit
Strain : other: Albino
Sex : male/female
Number of animals : 4
Vehicle : other: none
Doses : 50, 200, 794, 3160 mg/kg (single dose)
Method : other
Year : 1964
GLP : no
Test substance :

Remark : In the highest dose group, two deaths occurred at 24 and 48 hours after exposure to the test substance. Death was preceded by marked depression, severe, dyspnea, prostration, excessive urination, and coma. Necropsy revealed congestion of the lungs, adrenals, kidneys, and blanched areas on the liver and spleen. In addition, inflammation of the bladder and gastrointestinal tract were noted. In the 794 mg/kg group, three of the four animals exhibited slight depression, dyspnea, unsteady gait with slight sprawling of the limbs at 24 hours after exposure to the test substance. However, by the third day post-exposure, all of the animals appeared normal. At the termination of the study, necrotic tissue was seen in the abdominal skin at the site of application of the test substance. Otherwise, no gross pathology was observed. In animals exposed to 50 and 200 mg/kg of the test substance, no signs of systemic toxicity were observed. These animals exhibited normal weight gain, appearance, and behavior.

Dermal irritation was noted at all dose levels and was characterized by

slight, transient erythema, edema, atonia, and desquamation at the lowest level. There was a dose-dependent increase in the intensity and persistence with pronounced irritation at the highest dose levels characterized by blanching, eschar formation, and necrosis.
Route of administration: Dermal
Frequency of Treatment: Single Dose
Dose/Concentration Levels: 50, 200, 794, 3160 mg/kg
Control group and Treatment: None

Result : LD50 = 3160 mg/kg
Test condition : Undiluted test sample was applied to clipped, intact abdominal skin under a dental dam binder. The trunk was subsequently wrapped with gauze and adhesive tape. Following a 24-hour exposure period, binders were removed and the abdominal area was sponged with corn oil to remove sample residue. Following exposure, animals were observed for mortality or toxic effects at 1, 4, and 24 hours, and once daily thereafter for a total of 14 days. A necropsy was performed on any animal that died during the study. At the end of the 14-day observation period, all surviving animals were weighed, sacrificed, and necropsied.
Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion : Under conditions of this study, Propanoic acid, 2,2-dimethyl- has a low order of acute dermal toxicity in rabbits.
Reliability : (2) valid with restrictions
Study performed Pre-GLP.
Flag : Critical study for SIDS endpoint
18.09.2006 (6)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration :
Exposure : Semiocclusive
Exposure time : 24 hour(s)
Number of animals : 4
Vehicle : other: none
PDII :
Result :
Classification :
Method :
Year : 1964
GLP : no
Test substance :

Remark : Dose/Concentration Levels: 50, 200, 794, 3160 mg/kg
Control group and Treatment: None

Route of administration: Dermal
Frequency of Treatment: Single Dose

Dermal irritation was noted at all dose levels and was characterized by slight, transient erythema, edema, atonia, and desquamation at the lowest level. There was a dose-dependent increase in the intensity and persistence with pronounced irritation at the highest dose levels characterized by blanching, eschar formation, and necrosis.

In the highest dose group, two deaths occurred at 24 and 48 hours after exposure to the test substance. Death was preceded by marked

depression, severe, dyspnea, prostration, excessive urination, and coma. Necropsy revealed congestion of the lungs, adrenals, kidneys, and blanched areas on the liver and spleen. In addition, inflammation of the bladder and gastrointestinal tract were noted. In the 794 mg/kg group, three of the four animals exhibited slight depression, dyspnea, unsteady gait with slight sprawling of the limbs at 24 hours after exposure to the test substance. However, by the third day post-exposure, all of the animals appeared normal. At the termination of the study, necrotic tissue was seen in the abdominal skin at the site of application of the test substance. Otherwise, no gross pathology was observed. In animals exposed to 50 and 200 mg/kg of the test substance, no signs of systemic toxicity were observed. These animals exhibited normal weight gain, appearance, and behavior.

Test condition : Undiluted test sample was applied to clipped, intact abdominal skin under a dental dam binder. The trunk was subsequently wrapped with gauze and adhesive tape. Following a 24-hour exposure period, binders were removed and the abdominal area was sponged with corn oil to remove sample residue. Following exposure, animals were observed for mortality or toxic effects at 1, 4, and 24 hours, and once daily thereafter for a total of 14 days. A necropsy was performed on any animal that died during the study. At the end of the 14-day observation period, all surviving animals were weighed, sacrificed, and necropsied.

Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-

Reliability : (2) valid with restrictions
Study performed Pre-GLP.

Flag : Critical study for SIDS endpoint

18.09.2006 (6)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration :
Dose :
Exposure time :
Comment : not rinsed
Number of animals : 6
Vehicle : none
Result :
Classification :
Method :
Year : 1964
GLP : no
Test substance :

Remark : The test substance produced eye irritation consisting of a moderate conjunctivitis in all animals at one hour, that gradually diminished in severity and was last observed on the fourth day; slight iritis in two animals, persisting for 24 hours; transient dullness in one rabbit and opacity of the cornea in another rabbit with some sloughing of corneal epithelium at 24 and 48 hours. All signs of irritation disappeared after the fourth day.

Test condition : Animals were individually housed in stainless steel cages, with adequate food and water.

The test material was administered as a single instillation of 0.1 ml into the lower conjunctival sac of the left eye of each animal. The upper and lower lids were gently held together for approximately 1 second to prevent loss of the material. The contralateral eye served as the control.

The eyes of each animal were examined 24, 48, and 72 hours, and 4, 7 and 10 days after administration. At each interval the treated and control

eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale.

Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Reliability : (2) valid with restrictions
Study performed pre-GLP.
Flag : Critical study for SIDS endpoint
16.10.2006 (6)

5.3 SENSITIZATION

Type :
Species : guinea pig
Number of animals :
Vehicle :
Result : not sensitizing
Classification :
Method : other: Magnusson, B. Kligman, A.M. J. Invest Dermatol., 52, 1969
Year : 1977
GLP : no
Test substance :

Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion : Not likely to be a skin sensitizer.
Reliability : (2) valid with restrictions
Although the original data was not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag : Critical study for SIDS endpoint
21.09.2006 (18)

5.4 REPEATED DOSE TOXICITY

Type :
Species : rabbit
Sex : male
Strain : other: Albino
Route of admin. : dermal
Exposure period :
Frequency of treatm. : 10 applications with a two-day rest between the 5th and 6th applications
Post exposure period :
Doses : 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol
Control group : other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application.
NOAEL : = 300 mg/kg
Method : other
Year : 1964
GLP : no
Test substance :

Remark : No. of animals/sex/dose: 4
Route of administration: Dermal
Vehicle: Isopropyl Alcohol (IPA)
Statistical method: Not reported
The control animals exhibited normal appearance and behavior throughout the study with the exception of nasal discharge in one animal and diarrhea in another. Slight body weight loss was observed during the first week, but the animals regained the weight and most animals showed overall weight gains by the end of the study. No treatment-related effects were observed

at gross necropsy. Repeat applications did not cause any histopathological alterations to the liver or kidney of the rabbits.

Control animals exhibited slight erythema throughout the study and slight atonia and desquamation following the fifth application. Animals that received the test substance exhibited normal appearance and behavior throughout the study. Animals in the low dose group showed a net body weight gain by the end of the study and animals in the high dose group showed a slight weight loss by the end of the study. Gross pathological findings revealed parasitic infection of the liver and pitted kidneys in one rabbit, congested lungs in another, and congestion in the pancreas and kidney of a third rabbit. Slight to moderate erythema was observed in the low dose animals. Animals in the high dose group displayed moderate erythema, moderate edema, and moderate to marked atonia and desquamation. Three of the animals in the high dose group had areas of necrosis that persisted through the study.

Result : For systemic effects: NOAEL = 300 mg/kg
Propanoic acid, 2,2-dimethyl- produced moderate to severe skin irritation.

Test condition : The test material was applied to clipped abdominal skin. A loose gauze binder or a collar was used to prevent ingestion of the test substance. Animals were housed individually and allowed free access to food and water. Each animal was weighed, sacrificed, and necropsied 24 hours after the final application of test material. At the beginning of the study and prior to the final application, the following clinical parameters were evaluated: total erythrocyte count, total and differential leukocyte count, hematocrit, and urinalysis. Histological analysis was performed on sections of liver and kidney. Sections of brain, thyroid, lungs, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved for possible future analysis.

Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-

Conclusion : Under the conditions of this study, Propanoic acid, 2,2-dimethyl- has a low order of systemic toxicity following repeated dermal exposure.

Reliability : (2) valid with restrictions
Study performed Pre-GLP

Flag : Critical study for SIDS endpoint

18.09.2006 (10)

Type :
Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period :
Frequency of treatm. : 28 consecutive days
Post exposure period :
Doses : 0, 10, 30, 100, and 300 mg/kg/day
Control group : other: Water/polyethylene glycol 200 50/50 (v/v) was administered to 14 animals.
NOAEL : = 300 - mg/kg
Method : OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year : 1990
GLP : yes
Test substance :

Remark : No treatment related effect on body weight, food intake, hematological parameters or histopathological observations. The only clinical signs seen in this study was a shaking of their heads and sneezing, producing a dark nasal discharge, immediately after dosing 100 and 300 mg/kg/day. This behavior probably resulted from a mild irritant effect of the volatile acidic test compound.

Slight increase of plasma alkaline phosphatase, cholesterol and bilirubin levels at the 100 and 300 mg/kg/day dose levels, and slight increase of alkaline phosphatase and cholesterol levels in the plasma at 30 mg/kg/day in females. Increase in kidney and liver weight by 300 mg/kg/day. None of these changes correlated with histopathology effects and were due to local irritation and increase in functional demand.

Number of animals: 7/sex/dose

Vehicle: Water/polyethylene glycol 200 50/50 (v/v)

Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion : Propanoic acid, 2,2-dimethyl- has a low order of sub-chronic toxicity.

No evidence of a cumulative toxic effect at any dose level. Transient post dosing nasal irritation and other slight adaptive changes (organ weight, clinical chemistry) were seen at 300, 100 and 30 mg/kg/day.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
18.09.2006 (20)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : other: Ames - bacterial reverse mutation assay
System of testing : Ames Salmonella assay with and without metabolic activation and E.coli
Test concentration : 0.01, 2, 20, 500, or 2000µg/plate ± S9. All diluted in DMSO
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method :
Year : 1978
GLP : no
Test substance :

Remark : Plate incorporation assay

Species/strain: Rat liver (S9) fraction

Induced: Aroclor 1254 induced (treatment not specified)

Result : There was no increase in reverse mutation rate in either the presence or absence of S9.
Test substance : CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion : Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay.
Reliability : (2) valid with restrictions
Although the original data was not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag : Critical study for SIDS endpoint
21.09.2006 (19)

Type : Yeast gene mutation assay
System of testing : other: Yeast with and without metabolic activation
Test concentration : 0.01, 0.1, 0.5, 1.0, 5.0 mg/ml ± S9. All diluted in DMSO
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method :
Year : 1978
GLP : no
Test substance :

Remark	:	Liquid suspension assay Species/strain: Saccharomyces cerevisiae JD1 Species/cell type: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) Statistical methods were not reported
Result	:	There was no increase in the mitotic gene conversion frequency in either the presence or absence of S9.
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion	:	Propanoic acid, 2,2-dimethyl- is not mutagenic in Saccharomyces cerevisiae JD1 under conditions of this assay.
Reliability	:	(2) valid with restrictions Although the original data was not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.

21.09.2006 (19)

Type	:	Chromosomal aberration test
System of testing	:	Cultured rat liver cell line
Test concentration	:	0, 125, 250, 500 µg/ml ± S9. All diluted in DMSO
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	1978
GLP	:	no
Test substance	:	
Remark	:	Rat liver cells (RL1) with and without metabolic activation. Rat liver cells were cultured with test substance at concentrations of 0-500 µg/ml for 24 hours. Cultures were processed for chromosome analyses and 100 cells analyzed from each of 3 cultures/dose group. Species/cell type: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) Statistical methods not reported.
Result	:	The top dose level resulted in 50% inhibition of cell growth in the presence of S9. There was no increased incidence of chromosome aberrations in the treated cells.
Test substance	:	CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion	:	Propanoic acid, 2,2-dimethyl- is not genotoxic in rat liver cells in vitro under conditions of this assay.
Reliability	:	(2) valid with restrictions Although the original data was not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

21.09.2006 (19)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 95823-36-2
CAS No.	:	95823-36-2
TSCA Name	:	Carboxylic acids, C6-8-neo-
Molecular Formula	:	Unspecified
Producer related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001
Substance related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001
Status	:	
Memo	:	ExxonMobil Chemical Company (EMCC) Neoacids - HPV
Printing date	:	06.11.2006
Revision date	:	
Date of last update	:	19.10.2006
Number of pages	:	36
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Neoacids C5 to C28 Category is a group of Neoacids whose physicochemical and toxicological properties are very similar and follow a regular pattern as a result of synthesis and structural similarity. The production of neoacid products involves the reaction between a branched olefin with carbon monoxide and water at elevated temperatures and pressures in the presence of an acid catalyst. The products in this category range in carbon number from C5 to C28.

The six substances share relatively similar physico-chemical properties, which suggests that their environmental fate will be similar. Neoacids are trialkylacetic acids in which each hydrogen on the non carboxyl carbon of acetic acid has been replaced by an alkyl group. There is also a likelihood of common precursors and breakdown products that can result in structurally similar metabolites (e.g. carboxylic acid). Because these substances are similar with regard to environmental behavior/effects and human health, consideration of these substances as a category is justified.

The category also contains propanoic acid, 2,2-dimethyl-, methyl ester (CAS#: 598-98-1). This material is an ester that is rapidly hydrolyzed to the parent neoacid - propanoic acid, 2,2-dimethyl- (CAS#: 75-98-9). Because of this rapid hydrolysis, propanoic acid, 2,2-dimethyl-, methyl ester has properties for health effects, aquatic toxicity, and environmental fate that are consistent with the neoacids.

01.09.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C7H14O2
Molecular weight : 130.19
Petrol class :

Flag : Critical study for SIDS endpoint
26.09.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid

Purity :
Colour :
Odour :

Remark : CAS Registry Number, Name, and General Structure for Members of the Neoacids C5 to C28 Category and Analogue Substances:

CAS RN: 95823-36-2
TSCA Name: Carboxylic acids, C6-8-neo-
R length (C number): C7
Structure of R: Linear
Category Member: Yes

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1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

2-ethyl-2-methylbutanoic acid

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neoheptanoic acid

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1.3 IMPURITIES

Purity : typical for marketed substance
CAS-No : 95823-36-2
EC-No :
EINECS-Name :
Molecular formula : C7H14O2
Value : = 97 % w/w

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1.4 ADDITIVES

Purity type : typical for marketed substance
CAS-No : 95823-36-2
EC-No :
EINECS-Name :
Molecular formula : C7H14O2
Value :
Function of additive :

Remark : No additives present
26.09.2006

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Chemical industry: used in synthesis

Remark : Primarily used as a component of synthetic lubricants or hydraulic fluids.
26.09.2006

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 24.6 °C
Sublimation	:	
Method	:	other: ASTM D97
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

26.09.2006 (14)

2.2 BOILING POINT

Value	:	= 207 - 210 °C at
Decomposition	:	
Method	:	other: D1078/01
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

26.09.2006 (14)

2.3 DENSITY

Type	:	density
Value	:	= .93 g/cm³ at 20 °C
Method	:	
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

27.09.2006 (14)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .325 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential vapor pressure for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

27.09.2006 (5)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 2.4 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential partition coefficient for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

27.09.2006 (5)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 1912 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	4.7 at 25 °C
Description	:	
Stable	:	
Deg. product	:	

Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	

Method	:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential water solubility for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

27.09.2006 (5)

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2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 97 °C
Type	:	closed cup
Method	:	other: TCC ASTM D56
Year	:	2003
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.
Flag	:	Critical study for SIDS endpoint

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2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	4.7
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions The value was calculated based on the chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

27.09.2006 (16)

2.13 VISCOSITY

Value	:	= 9 - at 20 °C
Result	:	
Method	:	other: ASTM D445
Year	:	2003
GLP	:	
Test substance	:	
Remark	:	Value measured in cSt
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.

27.09.2006 (14)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000033 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year	:	2003
GLP	:	
Test substance	:	

Result :

Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (days)	OH- Rate Constant (cm3/molecule-sec)
3.2	3.2965 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C

Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : CAS No. 95823-36-2; Carboxylic acids, C6-8-neo

Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.

Flag : Critical study for SIDS endpoint
27.09.2006 (5)

Type : water
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
Deg. product :
Method : other (calculated): Technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterizing the potential of substances in the Neoacids C5 to C28 Category to undergo direct photodegradation.

Result : Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Neoacids C5 to C28 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References:

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Boethling, R.S., Mackay, D. 2000. Handbook of Property Estimation Methods for Chemicals, CRC Press, Boca Raton, FL, USA.

Test substance : Neoacids C5 to C28 Category members
Flag : Critical study for SIDS endpoint
01.09.2006 (4)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method : other: technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterising the potential of substances in the Neoacids C5 to C28 Category to undergo hydrolysis.
Result : Hydrolysis as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

Chemicals that are susecptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances 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). The lack of a suitable leaving group renders a compound resistant to hydrolysis.

Aliphatic acids are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982).

References:

Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

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.

Test substance : Neoacids C5 to C28 Category members
Conclusion : Hydrolysis will not contribute to the removal of neoacids from the environment.

Flag : Critical study for SIDS endpoint
01.09.2006 (3)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 130.19 g/mol
Water solubility = 1912 mg/L
Vapour pressure = 32.5 Pa
log Kow = 2.4
Melting point = 24.6 deg C

Degradation half-lives:

Air - 38.9 hrs
Water - 720 hrs
Soil - 7200 hrs
Sediment - 72000 hrs

This model was run assuming 100% discharge to water.

Result :

Air - 0.71%
Water - 98.2%
Soil - 0.39%
Sediment - 0.74%

Test substance : CAS No. 95823-36-2; Carboxylic acids, C6-8-neo

Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
27.09.2006		(17)
Type	:	fugacity model level I
Media	:	other: air - biota - sediment(s) - soil - water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation according Mackay, Level I
Year	:	2003
Method	:	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. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). Input values used: Molecular mass = 130.19 g/mol Water solubility = 1912 mg/L Vapour pressure = 32.5 Pa log Kow = 2.4 Melting point = 24.6 deg C
Result	:	Soil - 13.3% Air - 26.7% Water - 59.7% Sediment - 0.3% Suspended Sed - <0.01% Biota - <0.01%
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Conclusion	:	Results of the Mackay Level I environmental distribution model suggest that Neoacids C5 to C28 Category substances have a potential to partition to soil and air. However, category members are weak organic acids with estimated dissociation constants (pKa) of 4.6 to 4.9 (Karickoff, et. al. 1991). Consequently, category substances at neutral pH, which is typical of most natural surface waters, are expected to dissociate (>99%) to the ionized form and therefore, remain largely in water. The Mackay model is usually limited to non-ionic organics and according to Harris and Hayes, 1982, the ionized species of organic acids are generally adsorbed by soils and sediments to a much lesser degree than are the neutral forms. As a result the Mackay model may overestimate the partitioning of Neoacids C5 to C28 Category substances to the soil and sediment compartments.
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
27.09.2006		(17)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge, domestic
Contact time	:	28 day(s)
Degradation	:	= 44 (±) % after 28 day(s)
Result	:	inherently biodegradable
Deg. product	:	
Method	:	OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year	:	1996
GLP	:	yes
Test substance	:	
Remark	:	Test Type: Manometric Respirometry Test
Result	:	Test material was not readily biodegradable. Half-life was not reached. By day 28, 44% degradation of the test material was observed. 10% biodegradation was achieved on day 19 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	62.8, 24.6, 44.6	44.0
Na Benzoate	98.9, 95.5	97.2

* replicate data

Test condition	:	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 between 31 and 50 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.
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Conclusion	:	Test substance is considered not readily biodegradable.
Reliability	:	(1) valid without restriction Code 1, Reliable without Restrictions
Flag	:	Critical study for SIDS endpoint

27.09.2006 (10)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF	:	= 3.16
Elimination	:	
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Calculated values using BCFWIN version 2.13, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	BCFWIN estimates the bioconcentration factor (BCF) of an organic compound using the compound's log octanol-water partition coefficient (Kow). The estimation methodology used by BCFWIN is described in "Improved Method for Estimating Bioconcentration Factor (BCF) from Octanol-Water Partition Coefficient", SRC TR-97-006 (2nd Update), July 22, 1997. Log Kow used = 2.43
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential bioaccumulation factor for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

27.09.2006 (5)

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
LC50	:	= 630 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	EPA OTS 797.1400
Year	:	1993
GLP	:	yes
Test substance	:	
Remark	:	Statistical Method: Graphical (EPA-600/4-90-027)
Result	:	LC50 = 630mg/L, based upon measured concentrations. Analytical method used was GC-FID Nominal Conc. Measured Conc. % Mortality @ 96 hr. Control <0.79 mg/L 0 56.25 mg/L 51.4 mg/L 0 112.5 mg/L 124 mg/L 0 225 mg/L 200 mg/L 0 450 mg/L 436 mg/L 0 900 mg/L 882 mg/L 0
Test condition	:	A stock solution of 900mg/L was prepared daily and administered via a stainless steel and glass proportional diluter to achieve the desired study concentrations. The stock solution was mixed for 30 minutes and adjusted to a pH of 7.5 +/- 0.1 as needed. All test material went into solution. The test chambers were duplicate 1L glass dishes located within 19L glass aquaria with a flow rate of 6 dish volumes per day. Each dish contained 10 fish. Test temperature was 22.8 Deg C., Lighting was 16 hours light : 8 hours dark with 51.8 to 52.9 ft-candles during full daylight periods. Dissolved Oxygen at initiation ranged from 8.4 to 8.5 mg/L and from 6.6 to 8.0 mg/L at termination. The pH was ranged from 7.6 to 7.2 during the study. Fish Mean Wt.= 0.065g. Mean Total length = 1.6cm, Test Loading = 0.11 g of fish/L.
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Conclusion	:	Test substance is considered low toxicity.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

27.09.2006 (11)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	flow through
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 138 measured/nominal
Limit Test	:	no
Analytical monitoring	:	yes
Method	:	EPA OTS 797.1300

Year	:	1993
GLP	:	yes
Test substance	:	
Result	:	LC50 = 138mg/L (Conf. limits 112 - 172), based upon measured concentrations. Analytical method used was GC-FID Nominal Conc. Measured Conc. % Immobilized @ 48 hr. Control <0.82 mg/L 10 56.25 mg/L 54.7 mg/L 0 112.5 mg/L 107.0 mg/L 35 225 mg/L 222.0 mg/L 90 450 mg/L 476.0 mg/L 100 900 mg/L 903.0 mg/L 100 Statistical Method = Probit (Finney) of SAS
Test condition	:	A stock solution of 900mg/L was prepared daily and administered via a stainless steel and glass proportional diluter to achieve the desired study concentrations. The stock solution was mixed for 30 minutes and adjusted to a pH of 7.5 +/- 0.1 as needed. All test material went into solution. The test chambers were duplicate 250ml glass dishes with 5cm Nytex screening attached to the top rim of the dish. The test vessels were located within 15 gal glass aquaria with a flow rate of 7 dish volumes per day. Each dish contained 10 test organisms. Test temperature was 20.9 Deg C., Lighting was 16 hours light : 8 hours dark with 51.6 to 53.0 ft-candles during full daylight periods. Dissolved Oxygen at initiation ranged from 8.1 to 8.2 mg/L and from 7.6 to 8.7 mg/L at termination. The pH was ranged from 7.4 to 7.6 during the study. Test organisms were <24 hrs at initiation from 15 day old adults.
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (read across from Heptanoic C7 acid - approximately 70% n-heptanoic acid, 30% iso-heptanoic acid).
Conclusion	:	Test substance is considered low toxicity
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

27.09.2006 (1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	
Exposure period	:	72 hour(s)
Unit	:	mg/l
NOEC	:	= 3 measured/nominal
LOEC	:	= 6.2 measured/nominal
EC50	:	= 6.49 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	other: US EPA TSCA 40 CFR792.1989
Year	:	1993
GLP	:	yes
Test substance	:	

Remark : Statistical Method: Linear Interpolation
Result : 96 hour EC50 = 6.49mg/L (95% CI 5.64 to 7.54) based upon initial measured values (day 0).

96 hour NOEC = 3.03mg/L based on initial measured values (day 0).

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID).

Nominal Conc. (mg/L)	Measured Conc. Day 0 (mg/L)	Mean Cells at 96 hr	% Inhibition at 96 hr
Control	0	2.3 E6	-
3.12	3.03	2.3 E6	0
6.25	6.20	1.2 E6	47.8
12.5	12.24	4.8 E5	79.1
25.0	23.55	4.2 E5	81.7
50.0	52.15	3.6 E5	84.3

Test condition : A 500mg/L stock solution was prepared by adding the appropriate amount of test substance to algal nutrient media in an aspirator bottle. The stock solution was mixed for 15 minutes at <10% vortex on a magnetic stir plate. After mixing the solution was drawn out the bottom port. The pH was adjusted to 7.5 +/- 0.1 as necessary. The stock was diluted with algal nutrient media to prepared test solutions. Three replicates and a media/toxicant blank were prepared for each concentration. Replicate vessels were 125ml autoclaved Erlenmeyer flasks sealed with gauze stoppers. Test flasks (except blanks) were inoculated with ~1.0E4 cells/ml of algae. All test vessels were placed on a shaker table at ~100 rpm during the study.

Nominal treatment levels were 8.0, 31.0, 62, 125, and 250mg/L

Test temperature was 23.9 Deg. C. Lighting was continuous at 399.8 to 411.65 ft candles. The pH was 7.5 at test initiation and ranged from 7.4 to 7.6 at test termination.

Test substance : CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Conclusion : Test substance is considered moderately toxic.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.10.2006 (9)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species : Daphnia magna (Crustacea)
Endpoint : other: adult immobilization
Exposure period : 21 day(s)
Unit : mg/l
NOEC : = 4.78 measured/nominal
LOEC : = 10.1 measured/nominal
EC50 : = 7.1 measured/nominal
Analytical monitoring : yes
Method : EPA OTS 797.1330
Year : 1993
GLP :

Test substance	:	
Result	:	The No Observed Effect Concentration (NOEC) and Lowest Observed Effect Concentration (LOEC) for Adult Immobilization was 4.78 and 10.1 mg/L, respectively. The NOEC and LOEC values for Offspring per Adult were 4.78 and 10.1 mg/L, respectively. The Maximum Acceptable Toxicant Concentration (MATC), which is the maximum concentration at which the test chemical can be present and not be toxic to the organism, was 6.93 mg/L, and was based on adult immobilization and number of young per adult. Statistical Methods = Probit (Finney) of SAS; and Duncan's Multiple Range Test of SAS.
Test condition	:	The study was conducted under flow-through conditions for a period of 21 days. A stock solution was prepared daily at a nominal concentration of 50 mg/L. The stock solution was delivered to the test chambers via a diluter system where it prepared test treatments at nominal levels of 0, 3.12, 6.25, 12.5, 25, and 50 mg/L. Measured concentrations were <0.9, 2.32, 4.78, 10.1, 21.7, and 44.4 mg/L. The flow of the solution through the test was equal to at least 6 times the volume of the test chambers in a 24-hour period. Test chambers were 250 ml glass bottles with nitex screen covers. Test organisms were fed green algae and a yeast/salmon starter/cereal leaves mixture daily. Forty daphnids (10 per 4 replicates) were tested at each concentration level. Solubility of C7 acid = 3200mg/l. Diluent Alkalinity = 35 mg CaCO3/l Hardness = 100 mg CaCO3/l Conductance = 236 umhos TOC = 1.1
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (read across from Heptanoic C7 acid - approximately 70% n-heptanoic acid, 30% iso-heptanoic acid).
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

27.09.2006 (2)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 1860 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	5
Vehicle	:	other: none
Doses	:	
Method	:	other
Year	:	1964
GLP	:	no
Test substance	:	
Remark	:	Route of administration: Gastric Intubation Frequency of Treatment: Single Dose Dose/Concentration Levels: 34.6, 120, 417, 1450, 5000, and 10000 mg/kg Control group and Treatment: None There were no principal toxic effects at 34.6, 120 and 417 mg/kg. In addition there were no findings at necropsy in these animals. At 1450 mg/kg, although there were no findings at necropsy, clinical signs were observed after dosing which included depression, dyspnea and slight to marked ataxia. At the two highest dose levels, all animals were dead within 24 hours. Prior to death, animals exhibited marked depression, sprawling of the limbs and depressed reflexes. Congestion of the lungs, kidneys and adrenals were observed in these animals.
Result	:	LD50= 1860 mg/kg
Test condition	:	The animals were fasted for a period of three to four hours prior to treatment. The animals were observed for toxic effects and mortality at one, four and 24 hours; and once daily thereafter for 14 days. Necropsy was performed on any animal that died. All surviving animals were weighed, sacrificed and necropsied.
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Conclusion	:	Under conditions of this study, Carboxylic acid, C6-8 neo acid has a low order of acute oral toxicity in rats.
Reliability	:	(2) valid with restrictions Study conducted Pre-GLP
Flag	:	Critical study for SIDS endpoint

27.09.2006 (7)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 3 mg/l
Species	:	rat
Strain	:	other: Albino
Sex	:	male
Number of animals	:	10
Vehicle	:	other: none
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other: NA
Year	:	1964

GLP	:	no
Test substance	:	
Remark	:	No significant toxic signs were observed during the 6-hour exposure period. All rats appeared normal up to 5 days following exposure. No deaths occurred rats throughout the study and no significant observations were made at necropsy. Route of administration: Inhalation Frequency of Treatment: Single 6-hour exposure Dose/Concentration Levels: Saturated vapors - the mean nominal concentration was 3.0 mg/L. Control group and Treatment: Groups of rats that served as common controls for the substances tested in this study were sacrificed and examined grossly.
Result	:	LC50 > 3.0 mg/L
Test condition	:	An atmosphere of saturated vapors was produced by forcing air through a bubbler system that contained the test substance. 31 ml of liquid was vaporized at a flow rate of 27 L/min. Animals were caged in wire mesh compartments within the exposure chamber. Animals were observed for mortality and toxic effects at 30-minute intervals during exposure and daily thereafter. The animals were observed for two weeks following exposure, at which point animals were sacrificed and necropsied. Any animals that died during the exposure or observation periods were necropsied.
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Conclusion	:	Under conditions of this study, Carboxylic acid, C6-8 neo has a low order of acute inhalation toxicity in rats.
Reliability	:	(2) valid with restrictions No vapor concentration verification (analytical), study conducted pre-GLP.
Flag	:	Critical study for SIDS endpoint

27.09.2006 (6)

Type	:	LC50
Value	:	> 3 mg/l
Species	:	mouse
Strain	:	other: Albino
Sex	:	male
Number of animals	:	10
Vehicle	:	other: none
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other: NA
Year	:	1964
GLP	:	no
Test substance	:	
Remark	:	No significant toxic signs were observed during the 6-hour exposure period. All mice appeared normal up to 5 days following exposure, when the mice developed uticaria. No deaths occurred in mice throughout the study and no significant observations were made at necropsy. Route of administration: Inhalation Frequency of Treatment: Single 6-hour exposure Dose/Concentration Levels: Saturated vapors - the mean nominal concentration was 3.0 mg/L. Control group and Treatment: Groups of mice that served as common controls for the substances tested in this study were sacrificed and examined grossly.
Result	:	LC50 > 3.0 mg/L
Test condition	:	An atmosphere of saturated vapors was produced by forcing air through a bubbler system that contained the test substance. 31 ml of liquid was vaporized at a flow rate of 27 L/min. Animals were caged in wire mesh compartments within the exposure chamber. Animals were observed for mortality and toxic effects at 30-minute intervals during exposure and daily

thereafter. The animals were observed for two weeks following exposure, at which point animals were sacrificed and necropsied. Any animals that died during the exposure or observation periods were necropsied.

Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Conclusion	:	Under conditions of this study, Carboxylic acid, C6-8 neo has a low order of acute inhalation toxicity in mice.
Reliability	:	(2) valid with restrictions No vapor concentration verification (analytical), study performed pre-GLP.
Flag	:	Critical study for SIDS endpoint

27.09.2006 (6)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 3160 mg/kg bw
Species	:	rabbit
Strain	:	other: Albino
Sex	:	male/female
Number of animals	:	4
Vehicle	:	other: none
Doses	:	
Method	:	other
Year	:	1964
GLP	:	no
Test substance	:	

Remark : One death occurred in the 200 mg/kg group at 48 hours post-exposure, but this was not considered to be treatment-related, since no deaths occurred in any of the other treatment groups. Upon necropsy, cecal obstruction and a large amount of fluid in the abdominal cavity were found. No signs of systemic toxicity were seen in any of the animals exposed to 50, 200, or 794 mg/kg. In the highest dose group, marked depression, dyspnea, ataxia, and sprawling of the limbs were observed 1 to 4 hours after application. However, the animals had completely recovered by 24 hours following exposure and exhibited normal appearance and behavior for the remainder of the 14-day post-exposure period. Necropsy revealed no significant signs of gross pathology in these animals.

Dose-dependent dermal irritation occurred at all of the doses tested. This ranged from slight to moderate erythema, atonia, and desquamation at the lower dose levels to moderate erythema and edema with atonia and desquamation at the two higher dose levels.
Route of administration: Dermal
Frequency of Treatment: Single Dose
Dose/Concentration Levels: 50, 200, 794, 3160 mg/kg
Control group and Treatment: None

Result	:	LD50 > 3160 mg/kg
Test condition	:	Undiluted test sample was applied to clipped, intact abdominal skin under a dental dam binder. The trunk was subsequently wrapped with gauze and adhesive tape. Following a 24-hour exposure period, binders were removed and the abdominal area was sponged with corn oil to remove sample residue. Following exposure, animals were observed for mortality or toxic effects at 1, 4, and 24 hours, and once daily thereafter for a total of 14 days. A necropsy was performed on any animal that died during the study. At the end of the 14-day observation period, all surviving animals were weighed, sacrificed, and necropsied.
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Conclusion	:	Under conditions of this study, Carboxylic acid, C6-8 neo acid has a low order of acute dermal toxicity in rabbits.
Reliability	:	(2) valid with restrictions

Study performed Pre-GLP.

Flag : Critical study for SIDS endpoint

27.09.2006 (6)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	
Exposure	:	Semiocclusive
Exposure time	:	24 hour(s)
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	
Classification	:	
Method	:	
Year	:	1964
GLP	:	no
Test substance	:	

Remark : Dose/Concentration Levels: 50, 200, 794, 3160 mg/kg
Control group and Treatment: None

Route of administration: Dermal
Frequency of Treatment: Single Dose

Dermal irritation was noted at all dose levels and was characterized by slight, transient erythema, edema, atonia, and desquamation at the lowest level. There was a dose-dependent increase in the intensity and persistence with pronounced irritation at the highest dose levels characterized by blanching, eschar formation, and necrosis.

In the highest dose group, two deaths occurred at 24 and 48 hours after exposure to the test substance. Death was preceded by marked depression, severe, dyspnea, prostration, excessive urination, and coma. Necropsy revealed congestion of the lungs, adrenals, kidneys, and blanched areas on the liver and spleen. In addition, inflammation of the bladder and gastrointestinal tract were noted. In the 794 mg/kg group, three of the four animals exhibited slight depression, dyspnea, unsteady gait with slight sprawling of the limbs at 24 hours after exposure to the test substance. However, by the third day post-exposure, all of the animals appeared normal. At the termination of the study, necrotic tissue was seen in the abdominal skin at the site of application of the test substance. Otherwise, no gross pathology was observed. In animals exposed to 50 and 200 mg/kg of the test substance, no signs of systemic toxicity were observed. These animals exhibited normal weight gain, appearance, and behavior.

Test condition : Undiluted test sample was applied to clipped, intact abdominal skin under a dental dam binder. The trunk was subsequently wrapped with gauze and adhesive tape. Following a 24-hour exposure period, binders were removed and the abdominal area was sponged with corn oil to remove sample residue. Following exposure, animals were observed for mortality or toxic effects at 1, 4, and 24 hours, and once daily thereafter for a total of 14 days. A necropsy was performed on any animal that died during the study. At the end of the 14-day observation period, all surviving animals were weighed, sacrificed, and necropsied.

Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions Study performed Pre-GLP
Flag	:	Critical study for SIDS endpoint

27.09.2006 (6)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	not rinsed
Number of animals	:	6
Vehicle	:	
Result	:	
Classification	:	
Method	:	
Year	:	1964
GLP	:	no
Test substance	:	
Remark	:	Carboxylic acid, C6-8 neo (CAS# 95823-36-2) produced moderate to marked conjunctivitis which persisted for 4 to 14 days in all animals. Slight iritis was seen in all rabbits disappearing within 48 hours. Dullness and corneal opacity with apparent sloughing and vascularisation were observed in all animals, but these reactions disappeared by the fourth and seventh days in four of the six rabbits.
Test condition	:	Animals were individually housed in stainless steel cages, with adequate food and water. The test material was administered as a single instillation of 0.1 ml into the lower conjunctival sac of the left eye of each animal. The upper and lower lids were gently held together for approximately 1 second to prevent loss of the material. The contralateral eye served as the control. The eyes of each animal were examined 24, 48, and 72 hours, and 4, 7 and 10 days after administration. At each interval the treated and control eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale.
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Reliability	:	(2) valid with restrictions Study performed Pre-GLP.
Flag	:	Critical study for SIDS endpoint

27.09.2006 (6)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rabbit
Sex	:	male
Strain	:	other: Albino
Route of admin.	:	dermal
Exposure period	:	
Frequency of treatm.	:	10 applications with a two-day rest between the 5th and 6th applications.

Post exposure period	:	
Doses	:	55.4 mg/kg, 553.7 mg/kg
Control group	:	other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application.
NOAEL	:	= 553.7 mg/kg
Method	:	other
Year	:	1964
GLP	:	no
Test substance	:	
Remark	:	Animals in the low dose group showed normal appearance behavior throughout the study. With the exception of one animal that showed a slight weight loss, the animals in the low dose group showed an overall body weight gain. In the high dose group, 3 of the 4 animals displayed normal appearance and behavior and either maintained their weight or had a slight weight loss. From the fifth through the ninth application, the fourth animal had labored breathing, weight loss, and was found dead 24 hours after the final application. Upon necropsy, this animal had congested and emphysematous lungs in addition to hemorrhagic areas in the renal medulla. The death of this animal was deemed to be unrelated to the treatment. Gross pathology of the remaining animals of the high dose group did not reveal any abnormalities other than a slight parasitic infection in the liver of one of the rabbits. Repeat applications did not cause any histopathological alterations to the liver or kidney of the rabbits. In the low dose animals, slight erythema was observed during the first week, with slight to moderate atonia and desquamation that followed the third application and lasted through the study. At the highest dose, slight to moderate erythema was observed and slight to moderate edema was present from the second through the fifth applications. After the fourth application, moderate to marked atonia, desquamation, and slight fissuring was observed through the remainder of the study. All animals showed areas of necrosis at the application site and in two animals, the skin was hypersensitive to touch. No. of animals/sex/dose: 4/dose Vehicle: None Statistical method: Not reported
Result	:	For systemic effects: NOAEL = 553.7 mg/kg Carboxylic acid, C6-8 neo produced moderate to severe skin irritation.
Test condition	:	The test material was applied to clipped abdominal skin. A loose gauze binder or a collar was used to prevent ingestion of the test substance. Animals were housed individually and allowed free access to food and water. Each animal was weighed, sacrificed, and necropsied 24 hours after the final application of test material. At the beginning of the study and prior to the final application, the following clinical parameters were evaluated: total erythrocyte count, total and differential leukocyte count, hematocrit, and urinalysis. Histological analysis was performed on sections of liver and kidney. Sections of brain, thyroid, lungs, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved for possible future analysis.
Test substance	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo
Conclusion	:	Under the conditions of this study, Carboxylic acid, C6-8 neo has a low order or systemic toxicity following repeated dermal exposure.
Reliability	:	(2) valid with restrictions Study performed Pre-GLP.
Flag	:	Critical study for SIDS endpoint

27.09.2006 (15)

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type	:	One generation study
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	other: Dietary
Exposure period	:	
Frequency of treatm.	:	
Premating exposure period		
Male	:	
Female	:	
Duration of test	:	
No. of generation studies	:	
Doses	:	0, 1000, 5000, 7500, and 10,000 ppm in diet
Control group	:	other: 10/sex
Method	:	other
Year	:	1999
GLP	:	yes
Test substance	:	other TS: Isooctanoic Acid (CAS No. 25103-52-0)
Remark	:	No. of animals/sex/dose: 10/sex/dose Statistics: For the statistical analysis the percent of normal sperm were transformed by Bloom's transformation. All variables were analyzed by standard one-way analysis of variance (ANOVA). Residuals from the model were tested for normality by the Shapiro-Wilk. When there were differences in-group means based on the ANOVA, differences in means were tested using Duncan's multiple range test. There were signs of a slight palatability problem with the 7500 ppm and 10,000 ppm diets with the males and the 10,000 ppm diet with the females as indicated by decreases in mean food consumption during the early part of the first week of the study. This problem resolved itself by the second week of the study. However, during the first week of gestation and for the entire postpartum period, mean food consumption was significantly decreased in the 10,000 ppm group females. There were no treatment-related clinical in-life observations, gross postmortem observations, or organ weight effect in the parental animals during this study. In addition, there were no statistically significant effects on reproductive indices or sperm parameters. The offspring displayed no treatment-related effects on survival, clinical observations, time to developmental landmarks, or offspring postmortem observations. Statistically significant suppression of body weight gain was observed in the 10,000 ppm adult females on PPD 4 and 14 when compared with controls. There were statistically significant decreases in the 10,000 ppm group's male mean offspring body weights on PND 14, 21, and 28. There also was a statistically significant decrease in the 10,000 ppm females' mean offspring body weight on PND 14 and 28. These decreases in body weight in dams and offspring were transient and were thought to be related to decreased maternal food consumption.
Result	:	Maternal and Offspring NOAEL = 7500 ppm
Test condition	:	P1 males and females (10 animals/sex) were exposed to the test substance for 10 weeks prior to mating. One male and one female were

paired for up to 2 weeks. Beginning on GD 21, mated females were examined at least twice daily for signs of parturition. On PND 0, 1, 4, 7, 14 and 21 the offspring were counted, sexed and each live pup was weighed. Pups were counted and examined externally on a daily basis during the postnatal period. All animals were weighed and examined on PND 28, 35, 42, and 49 (males only were weighed and examined on PND Day 49). On PND 4, after counting, weighing, and examining the pups, the size of each litter was adjusted by eliminating extra pups by random selection to yield as nearly as possible, 4 males and 4 females per liter. Pups from each litter were examined daily for developmental landmarks. Sperm analyses were conducted at necropsy.
Surviving F1 females were sacrificed on PND 42 and surviving F1 males were sacrificed on PND 49 unless they had not met criteria for vaginal patency or preputial separation, respectively.

Test substance : Isooctanoic Acid (CAS No. 25103-52-0)
Conclusion : Under the conditions of this study Isooctanoic acid did not adversely affect reproductive parameters at doses that were nontoxic to the dams or their offspring.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
27.09.2006 (13)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : other: oral gavage
Exposure period : Days 6-15 of gestation
Frequency of treatm. :
Duration of test :
Doses : 0, 50, 250, 600, or 800 mg/kg
Control group : other: Controls received 800 mg/kg of distilled water
NOAEL maternal tox. : = 250 mg/kg bw
Method : OECD Guide-line 414 "Teratogenicity"
Year : 1986
GLP : yes
Test substance :

Remark : Number/sex/dose: 22/dose
Statistical methods: ANOVA, Kruskal-Wallis, Fisher's exact test
Result : NOAEL fetal: 250 mg/kg
NOAEL maternal: 250 mg/kg

Maternal:
The high dose of 800 mg/kg produced morbidity and mortality in 4 of the 22 mated females. This group displayed lethargy, abnormal breathing, rales, and staining around the muzzle and anogenital areas. Animals in the 600 mg/kg group had a significant incidence of rales. In the high dose group (800 mg/kg), maternal body weight gain and uterine weight at term were significantly reduced. In the 600 mg/kg group, there was a significant reduction in body weight gain during the intervals of gd6-9 and gd0-20. Maternal food consumption was significantly reduced during gestational intervals gd6-9 and gd9-12 for both the 600 and 800 mg/kg groups and during gd12-16 in the 800 mg/kg group.

Fetus:
In the high dose group, there was a significant increase in early embryonic resorptions with a corresponding decrease in the mean number of live fetuses. The remaining fetuses in the high dose group had significantly

reduced fetal body weight and crown-rump distance. Microphthalmia and anophthalmia were observed in 14% of the fetuses from the high dose group. In addition, fused cervical vertebrae and misaligned thoracic vertebra were observed in the high dose group. Significant incidences of hydrocephalus and structural malformation of thoracic ribs occurred in both the 600 and 800 mg/kg groups. The fraction of malformed fetuses/live fetuses was significantly increased in the 600 and 800 mg/kg groups. In the 250 mg/kg group, there was an increase in the fraction of implants affected, however, this was not significantly different from the control group.

Visceral examination revealed that the incidence of renal/ureter variations was significantly increased in the high dose group. In addition, the high dose group showed an increased incidence of unossified structures of the cranium, sternum, vertebrae, pelvis, and hindpaw. In both the 600 and 800 mg/kg groups, there were increases in the incidences of incompletely ossified supraoccipital and cervical vertebrae.

Test condition : Physical examinations were performed and body weight and food consumption were measured throughout gestation. Mated females were sacrificed on gestational day 20 and a gross necropsy was performed. Uteri and ovaries were weighed and corpora lutea were counted. The number of implantation sites, early and late resorptions, and live and dead fetuses were determined. Full term fetuses were examined for abnormalities, weight, and crown-rump distance. From each litter, the heads of half of the fetuses were preserved and examined, while the other half of the fetuses were examined for skeletal malformations and ossification variations.

Test substance : CAS No. 95823-36-2; Carboxylic acids, C6-8-neo

Conclusion : Carboxylic acid, C6-8 neo is embryo-lethal and teratogenic in rats at doses that are maternally toxic. Under the conditions of this study, Carboxylic acid, C6-8 neo is not a selective developmental toxicant.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

27.09.2006 (8)

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : other: oral gavage
Exposure period :
Frequency of treatm. :
Duration of test :
Doses : 0, 50, 200, 400, 800, and 1000 mg/kg/day
Control group : other: Vehicle control: corn oil
NOAEL maternal tox. : = 400 - mg/kg bw
Method : other
Year : 1995
GLP : yes
Test substance : other TS: Isooctanoic Acid (CAS No. 25103-52-0)

Remark : No. of animals/sex/dose: 25/dose
Vehicle: Corn oil
Statistical methods: Statistical evaluation of equality of means was done by appropriate one way analysis of variance. Also, a standard regression analysis for linear response in the dose groups was performed.

Result : Maternal NOAEL = 400 mg/kg/day
Fetal NOAEL = 800 mg/kg/day

Maternal: There were no treatment-related deaths during the study. However, there were some deaths in the different dose groups that were attributed to intubation errors. Animals in the 800 and 1000 mg/kg/day groups displayed clinical signs that included rales, stool abnormalities, and

anogenital/abdominal staining following dose initiation on GD6. Animals in the remaining dose groups were free of clinical signs for the entire gestation period. Overall, there were no statistically significant differences in mean body weight gain for the entire gestation interval or the entire gestation interval corrected for uterine weight between treated and control animals. However, in the 800 and 1000 mg/kg/day groups, there were statistically significant decreases in body weight gain early during gestation (GD 6-15). This correlated with decreased mean food consumption in these groups during this time frame. In the 400 mg/kg/day group, there was evidence of slight body weight gain suppression during the interval following dosing. However, these animals recovered quickly and in the absence of a consistent response, this finding was considered the result of slight dosing trauma. There were no significant findings at necropsy other than some trauma that was indicative of dosing errors.

Fetal: There were no statistically significant differences in reproductive parameters including: total live fetuses, sex ratio, mean number of resorptions, mean number of implantation sites, mean number of corpora lutea, mean fetuses per implantation site, mean resorptions per implantation site, % pre-implantation losses, % post-implantation loss, or mean total affected (resorptions + dead + malformed fetuses per litter) between treated and control animals. No external abnormalities were observed in any fetuses from the control or treated groups. In the highest dose group, a statistically significant decrease in mean male and female fetal body weights was observed compared with the controls.

Test condition : Males and females were housed together until confirmation of mating. The presence of a sperm plug was set as gestational day (GD) 0. Mated females were dosed once daily from GD 6-15. Dosing volumes were 5 ml/kg for all groups and were based on the most recent body weight. Clinical observations were made daily during gestation. Food consumption and body weight measurements were made on every three days through GD21. On GD21, animals were euthanized and cesarean sections were performed. Gross necropsies were performed, uterine weights with ovaries were measured, uterine contents were examined, and uterine implantation data were recorded. All live fetuses were weighed, examined externally to determine sex and for gross malformations.

Test substance : Isooctanoic Acid (CAS No. 25103-52-0)

Conclusion : Under the conditions of this study, Isooctanoic acid is not a selective developmental toxicant.

Reliability : (2) valid with restrictions
Study was performed as a range-finding study.

27.09.2006 (12)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) EMBSI (1993) Daphnia Acute Flow-through Toxicity Test. ExxonMobil Biomedical Sciences, Inc. Unpublished report.

(2) EMBSI (1994). Daphnia Sp. Chronic Flow-through Toxicity Test. ExxonMobil Biomedical Sciences, Inc. Unpublished report.

(3) EMBSI (2005) Hydrolysis: Neoacids C5 to C28 Category.

(4) EMBSI (2005) Photodegradation (Direct): Neoacids C5 to C28 Category.

(5) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(6) Esso Research and Engineering Company (1964).
Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.

(7) Esso Research and Engineering Company (1964).
Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.

(8) Exxon Biomedical Sciences (1986) "Oral teratology study in rats," Unpublished study.

(9) Exxon Biomedical Sciences Inc. Algal Acute Toxicity Test 148667.

(10) Exxon Biomedical Sciences Inc. Ready Biodegradability: OECD 301F Manometric Respirometry Test. 136894A.

(11) Exxon Biomedical Sciences, Inc. Fish Acute Flow-through Toxicity Test, 148641.

(12) Exxon Biomedical Sciences, Inc. (1995). "Developmental toxicity range-finding study in rats," Unpublished report.

(13) Exxon Biomedical Sciences, Inc. (1999) "One generation reproduction toxicity range-finding study in rats," Unpublished report.

(14) ExxonMobil Chemical Company (2003). Carboxylic acids, C6-8-neo. Unpublished internal data.

(15) Hazleton Laboratories, Inc. (1964) "Repeated Dermal Application - Rabbits," Unpublished report.

(16) Karickoff, S.W., V.K. McDaniel, C. Melton, A.N. Vellino, D.E. Nute, L.A. Carreira (1991). Predicting chemical reactivity by computer. Environ. Toxicol. Chem. 10:1405-1416.

(17) Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model ver. 2.02, available from the Environmental Centre, Trent University, Canada.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 26896-20-8
CAS No.	:	26896-20-8
EINECS Name	:	Neodecanoic acid
EC No.	:	248-093-9
Molecular Weight	:	173
Molecular Formula	:	C10H20O2

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001
Status	:	
Memo	:	ExxonMobil Chemical Company (EMCC) Neoacids - HPV
Printing date	:	06.11.2006
Revision date	:	
Date of last update	:	19.10.2006
Number of pages	:	39
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Neoacids C5 to C28 Category is a group of Neoacids whose physicochemical and toxicological properties are very similar and follow a regular pattern as a result of synthesis and structural similarity. The production of neoacid products involves the reaction between a branched olefin with carbon monoxide and water at elevated temperatures and pressures in the presence of an acid catalyst. The products in this category range in carbon number from C5 to C28.

The six substances share relatively similar physico-chemical properties, which suggests that their environmental fate will be similar. Neoacids are trialkylacetic acids in which each hydrogen on the non carboxyl carbon of acetic acid has been replaced by an alkyl group. There is also a likelihood of common precursors and breakdown products that can result in structurally similar metabolites (e.g. carboxylic acid). Because these substances are similar with regard to environmental behavior/effects and human health, consideration of these substances as a category is justified.

The category also contains propanoic acid, 2,2-dimethyl-, methyl ester (CAS#: 598-98-1). This material is an ester that is rapidly hydrolyzed to the parent neoacid - propanoic acid, 2,2-dimethyl- (CAS#: 75-98-9). Because of this rapid hydrolysis, propanoic acid, 2,2-dimethyl-, methyl ester has properties for health effects, aquatic toxicity, and environmental fate that are consistent with the neoacids.

01.09.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C10H20O2
Molecular weight : 172.27
Petrol class :

29.09.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid
Purity :

Colour :
Odour :

Remark : CAS Registry Number, Name, and General Structure for Members of the Neoacids C5 to C28 Category and Analogue Substances:

CAS RN: 26896-20-8
TSCA Name: Neodecanoic acid-
R length (C number): C10
Structure of R: Linear
Category Member: Yes

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1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

2,2-Dimethyloctanoic acid

19.11.2001

Neodecanoic Acid 10

29.09.2006

1.3 IMPURITIES

Purity : typical for marketed substance
CAS-No : 26896-20-8
EC-No : 248-093-9
EINECS-Name : neodecanoic acid
Molecular formula : C10H20O2
Value : > 97 % w/w

29.09.2006

1.4 ADDITIVES

Purity type : typical for marketed substance
CAS-No : 26896-20-8
EC-No : 248-093-9
EINECS-Name : neodecanoic acid
Molecular formula :
Value :
Function of additive :

Remark : No additives present
29.09.2006

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Chemical industry: used in synthesis
Remark	:	Primarily used as an intermediate in the production of drying agents, PVC stabilizers, and alkyd resins.

29.09.2006

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 57.1 °C
Sublimation	:	
Method	:	other: ASTM D97
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

29.09.2006 (11)

2.2 BOILING POINT

Value	:	= 250 - 257 °C at
Decomposition	:	
Method	:	other: D1078/01
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

29.09.2006 (11)

2.3 DENSITY

Type	:	density
Value	:	= .91 at 20 °C
Method	:	
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

29.09.2006 (11)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .009 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential vapor pressure for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

29.09.2006 (6)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 3.9 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential partition coefficient for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

29.09.2006 (6)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 69 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	4.8 at 25 °C
Description	:	
Stable	:	
Deg. product	:	

Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	

Method	:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential water solubility for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

29.09.2006 (6)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 122 °C
Type	:	open cup
Method	:	other: COC ASTM D92
Year	:	2003
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.
Flag	:	Critical study for SIDS endpoint

02.10.2006 (11)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	4.8
Method	:	other: calculated

Year	:	2003
GLP	:	
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions The value was calculated based on the chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

02.10.2006 (14)

2.13 VISCOSITY

Value	:	= 40 - at 20 °C
Result	:	
Method	:	other: ASTM D445
Year	:	2003
GLP	:	no data
Test substance	:	
Remark	:	Value measured in cSt
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.

02.10.2006 (11)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000075357 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year	:	2003
GLP	:	
Test substance	:	

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (days)	OH- Rate Constant (cm3/molecule-sec)
1.4	7.5357 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C

Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : CAS No. 26896-20-8; Neodecanoic acid
Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.
Flag : Critical study for SIDS endpoint
02.10.2006 (6)

Type : water
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
Deg. product :
Method : other (calculated): Technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterizing the potential of substances in the Neoacids C5 to C28 Category to undergo direct photodegradation.
Result : Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Neoacids C5 to C28 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References:

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Boethling, R.S., Mackay, D. 2000. Handbook of Property Estimation Methods for Chemicals, CRC Press, Boca Raton, FL, USA.

Test substance : Neoacids C5 to C28 Category members
Flag : Critical study for SIDS endpoint
01.09.2006 (5)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method : other: technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterising the potential of substances in the Neoacids C5 to C28 Category to undergo hydrolysis.
Result : Hydrolysis as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

Chemicals that are susecptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances 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). The lack of a suitable leaving group renders a compound resistant to hydrolysis.

Aliphatic acids are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982).

References:

Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

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.

Test substance : Neoacids C5 to C28 Category members
Conclusion : Hydrolysis will not contribute to the removal of neoacids from the environment.

Flag : Critical study for SIDS endpoint
01.09.2006 (4)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 172.27 g/mol
Water solubility = 69 mg/L
Vapour pressure = 0.95 Pa
log Kow = 3.9
Melting point = 57.1 deg C

Degradation half-lives:

Air - 17.0 hrs
Water - 240000 hrs
Soil - 720000 hrs
Sediment - 7200000 hrs

This model was run assuming 100% discharge to water.

Result :

Air - 0.28%
Water - 66.7%
Soil - 5.7%
Sediment - 27.3%

Test substance : CAS No. 26896-20-8; Neodecanoic acid

Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
02.10.2006		(15)

Type	:	fugacity model level I
Media	:	other: air - biota - sediment(s) - soil - water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation according Mackay, Level I
Year	:	2003
Method	:	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. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). Input values used: Molecular mass = 172.27 g/mol Water solubility = 69 mg/L Vapour pressure = 0.95 Pa log Kow = 3.9 Melting point = 57.1 deg C
Result	:	Soil - 81.1% Air - 5.5% Water - 11.5% Sediment - 1.8% Suspended Sed - 0.06% Biota - <0.01%
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Conclusion	:	Results of the Mackay Level I environmental distribution model suggest that Neoacids C5 to C28 Category substances have a potential to partition to soil and air. However, category members are weak organic acids with estimated dissociation constants (pKa) of 4.6 to 4.9 (Karickoff, et. al. 1991). Consequently, category substances at neutral pH, which is typical of most natural surface waters, are expected to dissociate (>99%) to the ionized form and therefore, remain largely in water. The Mackay model is usually limited to non-ionic organics and according to Harris and Hayes, 1982, the ionized species of organic acids are generally adsorbed by soils and sediments to a much lesser degree than are the neutral forms. As a result the Mackay model may overestimate the partitioning of Neoacids C5 to C28 Category substances to the soil and sediment compartments.
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
02.10.2006		(15)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge, domestic
Contact time	:	28 day(s)
Degradation	:	= 11 (±) % after 28 day(s)
Result	:	
Deg. product	:	
Method	:	OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year	:	1996
GLP	:	yes
Test substance	:	
Remark	:	Test Type: Manometric Respirometry Test
Result	:	Test material was not readily biodegradable. Half-life was not reached. By day 28, 11% degradation of the test material was observed. 10% biodegradation was achieved on day 27 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	20.5, 3.60, 8.90	11.0
Na Benzoate	98.9, 95.5	97.2

* replicate data

Test condition	:	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 between 31 and 50 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.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Conclusion	:	Test substance is considered not readily biodegradable.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

29.09.2006 (8)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF	:	= 3.16
Elimination	:	
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Calculated values using BCFWIN version 2.13, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	BCFWIN estimates the bioconcentration factor (BCF) of an organic compound using the compound's log octanol-water partition coefficient (Kow). The estimation methodology used by BCFWIN is described in "Improved Method for Estimating Bioconcentration Factor (BCF) from Octanol-Water Partition Coefficient", SRC TR-97-006 (2nd Update), July 22, 1997. Log Kow used = 3.90
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential bioaccumulation factor for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

02.10.2006 (6)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 37.2 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	1996
GLP	:	yes
Test substance	:	
Remark	:	Statistical Method: Bionomial Method
Result	:	LC50 = 37.2mg/L (CI 26.3 to 52.5), based upon measured concentrations of mean of old and new samples. Analytical method used was GC-FID. LL50 = 35.4 mg/L (CI 25.0 to 50.0), based upon nominal loading levels.

Nominal Conc.	Measured Conc.	% Mortality @ 96 hr.
Control	Below detection	0
6.25 mg/L	10.3 mg/L	0
12.5 mg/L	13.6 mg/L	0
25 mg/L	26.3 mg/L	0
50 mg/L	52.5 mg/L	0
100 mg/L	102 mg/L	0

Test condition	:	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 solution was mixed for 24 hours at a vortex of </= 10% of the total depth. After mixing the mixtures were adjust for pH to that of the dilution water using 1.0m NaOH. 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 19 hours light : 5 hours dark with 528 to 538 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.5 to 9.0 mg/L and from 5.9 to 7.4 mg/L in "old" solutions prior to renewals. The pH was ranged from 7.0 to 7.6 during the study. Fish were not fed during the study. Fish Mean Wt.= 0.260g. Mean Total length = 3.3cm, Test Loading = 0.29 g of fish/L.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Conclusion	:	Test substance is considered moderate toxicity.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

29.09.2006 (9)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
LL50	:	= 47.1
Analytical monitoring	:	no
Method	:	other: USEPA -660/3-75-009 Methods for Acute Toxicity with Fish and Macroinvertebrates, and Amphibians, 1975
Year	:	1977
GLP	:	no
Test substance	:	
Remark	:	Daphnid Acute Toxicity Test Statistical Method: Moving Average-Angle Method, (Harris 1959)
Result	:	LL50 = 47.1 mg/L (95% CI 33.6 to 57.8) based upon nominal test concentrations.

Mean % Mortality

Test Concentration	24 hr.	48 hr.
Positive Control	0	0
Negative Control	0	0
13 mg/L	0	13
22 mg/L	0	13
36 mg/L	0	20
60 mg/L	20	67
100 mg/L	53	100
170 mg/L	87	100
280 mg/L	73	100

Test condition	:	For each test concentration, the appropriate amount of test substance was dissolved in triethylene glycol (TEG) and pipetted into 500ml of dilution water. This solution was mixed with a magnetic stirrer and divided into three 150ml replicates for testing. The remaining 50ml was used for pH and dissolved oxygen measurements. A positive control (with TEG) and a negative control (dilution water) were also tested. Test vessels were 250ml beakers containing five daphnids each. Dilution water was reconstituted deionized well water with a hardness of 180mg/L as CaCO3, with a pH of 8.0. The test was performed under static conditions with no aeration. Nominal test concentrations were 13, 22, 36, 60, 100, 170, and 280 mg/L Test temperature was 22+/- 1 Deg C. Dissolved oxygen ranged from 8.6 to 8.8 mg/L during the study. The pH of the test solutions ranged from 7.1 to 8.2. Organisms were <24 hrs old, supplied by in-house cultures.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Conclusion	:	Test substance is considered to be of moderate toxicity.
Reliability	:	(2) valid with restrictions Lack of measured concentrations, no documentation of pH adjustment of treatments.
Flag	:	Critical study for SIDS endpoint

29.09.2006 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 2000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	5
Vehicle	:	other: none
Doses	:	34.6, 120, 417, 1450, 5000, and 10000 mg/kg
Method	:	other
Year	:	1964
GLP	:	no
Test substance	:	
Remark	:	Route of administration: Gastric Intubation Frequency of Treatment: Single Dose Dose/Concentration Levels: 34.6, 120, 417, 1450, 5000, and 10000 mg/kg Control group and Treatment: None There were no principal toxic effects or necropsy findings for animals in the 34.6, 120 and 417 mg/kg treatment groups. At 1450 mg/kg, 1 animal died within 24 hours of exposure and one animal died each day thereafter until all 5 animals were dead by day 5 of the study. Prior to death, slight to marked CNS depression, dyspnea, and ataxia was observed. In addition, congestion of the lungs, kidneys and adrenals were observed at necropsy. In the 5,000 mg/kg dose group, 2/5 animals died by 4 hours and 5/5 animals were dead by 24 hours following exposure. In the highest dose group, 4/5 animals died by 4 hours and all animals were dead by 24 hours post-treatment. Animals in the 5,000 and 10,000 mg/kg groups appeared to have depression, dyspnea, ataxia and sprawling of the limbs. Also at these two dose levels, necropsy findings indicated congestion of the lungs, liver, spleen, kidneys and adrenals.
Result	:	LD50= 2000 mg/kg
Test condition	:	The animals were fasted for a period of three to four hours prior to treatment. The animals were observed for toxic effects and mortality at one, four and 24 hours; and once daily thereafter for 14 days. Necropsy was performed on any animal that died. All surviving animals were weighed, sacrificed and necropsied.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid)
Conclusion	:	2,2-Dimethyloctanoic acid has a low order of acute oral toxicity in rodents.
Reliability	:	(2) valid with restrictions Study performed Pre-GLP
Flag	:	Critical study for SIDS endpoint

04.10.2006 (7)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 3 mg/l
Species	:	rat
Strain	:	Wistar
Sex	:	male
Number of animals	:	10
Vehicle	:	other: None

Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1964
GLP	:	no
Test substance	:	
Remark	:	No mortality or significant signs of toxicity were observed during the 6-hour exposure period. No deaths occurred in mice or rats throughout the study and no significant observations were made at necropsy. Route of administration: Inhalation Frequency of Treatment: Single 6-hour exposure Dose/Concentration Levels: Saturated vapors - the mean nominal concentration was 3.0 mg/L. Control group and Treatment: A group of mice and rats that served as a common control for the substances tested in this study were sacrificed and examined grossly.
Result	:	LC50 > 3.0 mg/L
Test condition	:	An atmosphere of saturated vapors was produced by forcing air through a bubbler system that contained the test substance. 20 ml of liquid was vaporized at a flow rate of 21 L/min. Animals were caged in wire mesh compartments within the exposure chamber. Animals were observed for mortality and toxic effects at 30-minute intervals during exposure and daily thereafter. The animals were observed for two weeks following exposure, at which point animals were sacrificed and necropsied. Any animals that died during the exposure or observation periods were also necropsied.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid)
Conclusion	:	Under conditions of this study, 2,2-Dimethyloctanoic acid has a low order of acute inhalation toxicity in mice and rats.
Reliability	:	(2) valid with restrictions No vapor concentration verification (analytical)

16.10.2006 (7)

Type	:	LC50
Value	:	> 511 mg/m³
Species	:	rat
Strain	:	Wistar
Sex	:	male/female
Number of animals	:	20
Vehicle	:	other: None
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1982
GLP	:	no
Test substance	:	
Remark	:	No animals died during the study. The control animals appeared normal throughout the exposure. During the two-week post-exposure period, incidences of ungroomed appearance, soft stool, and anogenital staining were observed in some of the control animals. One female guinea pig in the control group died on the fifth day of the post-exposure observation period. Animals exposed to the test material exhibited some signs of labored breathing, salivation, and eye irritation during the exposure. Upon removal from the chamber, exposed mice and guinea pigs had material-covered fur and exposed rats had some red staining around the nasal area, anogenital staining, soft stool, salivation, and lacrimation. During the two-week post-exposure observation period, all guinea pigs appeared normal. However, some of the mice appeared ungroomed and some rats exhibited anogenital staining and soft stool. Throughout the study, body weights remained

normal except for a slight weight loss on the first and second post-exposure days in both the control and treated groups (all species).

At terminal sacrifice, male mice exposed to the aerosolized test substance exhibited a statistically significant decrease in the liver to body weight ratio versus control animals. No other statistically significant differences were observed for group mean organ weight to body weight ratios. Minor macroscopic abnormalities were observed in both control and treated groups at the interim and terminal necropsies, but were not considered to be related to exposure to the test substance.
Route of administration: Inhalation
Frequency of Treatment: Single 6-hour exposure
Dose/Concentration Levels: Liquid aerosol with a mean analytical concentration of 511 mg/m3
Control group and Treatment: 10/sex/species

Result : LC50 > 511 mg/m3
Test condition : Groups of animals (10/sex/species) were exposed to either air only or to aerosolized test material. Aerosol was generated by pumping the test material into an atomizer at 15.0 psi. The resulting aerosol was sprayed into a glass aerosol diffuser, where it was mixed with incoming room air before entering the chamber. Exposure concentrations were determined on both a nominal and actual (gravimetric) basis. Particle size determinations were conducted twice during exposure. During the exposure, control and treated animals were observed every 15 minutes for the first hour and hourly thereafter. On the first day post-exposure, one half of the animals from each group were randomly selected and sacrificed, and an interim necropsy was performed. The remaining animals were observed daily for signs of toxicity for 14 days post-exposure. Body weights were recorded at the beginning of the study, and at 1, 2, 3, 4, 7, and 14 days post-exposure. A necropsy was performed on all animals that died or were sacrificed during the study. Major organs were examined for macroscopic abnormalities and lungs plus trachea, liver, kidneys, whole head, and any abnormal tissues were preserved. Organ weights were recorded at necropsy for lungs plus trachea, liver, and kidneys.
Test substance : CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid)
Conclusion : Under conditions of this study, aerosolized 2,2-Dimethyloctanoic acid has a low order of acute inhalation toxicity in mice, rats, and guinea pigs.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
04.10.2006 (1)

Type : LC50
Value : > 3 mg/l
Species : mouse
Strain : other: Swiss albino
Sex : male
Number of animals : 10
Vehicle : other: None
Doses :
Exposure time : 6 hour(s)
Method : other
Year : 1964
GLP : no
Test substance :

Remark : No mortality or significant signs of toxicity were observed during the 6-hour exposure period. No deaths occurred in mice or rats throughout the study and no significant observations were made at necropsy.
Route of administration: Inhalation
Frequency of Treatment: Single 6-hour exposure
Dose/Concentration Levels: Saturated vapors - the mean nominal concentration was 3.0 mg/L.

Control group and Treatment: A group of mice and rats that served as a common control for the substances tested in this study were sacrificed and examined grossly.

Result	:	LC50 > 3.0 mg/L
Test condition	:	An atmosphere of saturated vapors was produced by forcing air through a bubbler system that contained the test substance. 20 ml of liquid was vaporized at a flow rate of 21 L/min. Animals were caged in wire mesh compartments within the exposure chamber. Animals were observed for mortality and toxic effects at 30-minute intervals during exposure and daily thereafter. The animals were observed for two weeks following exposure, at which point animals were sacrificed and necropsied. Any animals that died during the exposure or observation periods were also necropsied.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid)
Conclusion	:	Under conditions of this study, 2,2-Dimethyloctanoic acid has a low order of acute inhalation toxicity in mice and rats.
Reliability	:	(2) valid with restrictions No vapor concentration verification (analytical)

16.10.2006 (7)

Type	:	LC50
Value	:	> 511 mg/m³
Species	:	mouse
Strain	:	other: Swiss albino
Sex	:	male/female
Number of animals	:	20
Vehicle	:	other: None
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1982
GLP	:	no
Test substance	:	

Remark :

No animals died during the study. The control animals appeared normal throughout the exposure. During the two-week post-exposure period, incidences of ungroomed appearance, soft stool, and anogenital staining were observed in some of the control animals. One female guinea pig in the control group died on the fifth day of the post-exposure observation period.

Animals exposed to the test material exhibited some signs of labored breathing, salivation, and eye irritation during the exposure. Upon removal from the chamber, exposed mice and guinea pigs had material-covered fur and exposed rats had some red staining around the nasal area, anogenital staining, soft stool, salivation, and lacrimation. During the two-week post-exposure observation period, all guinea pigs appeared normal. However, some of the mice appeared ungroomed and some rats exhibited anogenital staining and soft stool. Throughout the study, body weights remained normal except for a slight weight loss on the first and second post-exposure days in both the control and treated groups (all species).

At terminal sacrifice, male mice exposed to the aerosolized test substance exhibited a statistically significant decrease in the liver to body weight ratio versus control animals. No other statistically significant differences were observed for group mean organ weight to body weight ratios. Minor macroscopic abnormalities were observed in both control and treated groups at the interim and terminal necropsies, but were not considered to be related to exposure to the test substance.
Route of administration: Inhalation
Frequency of Treatment: Single 6-hour exposure
Dose/Concentration Levels: Liquid aerosol with a mean analytical concentration of 511 mg/m3

Control group and Treatment: 10/sex/species

Result : LC50 > 511 mg/m3

Test condition : Groups of animals (10/sex/species) were exposed to either air only or to aerosolized test material. Aerosol was generated by pumping the test material into an atomizer at 15.0 psi. The resulting aerosol was sprayed into a glass aerosol diffuser, where it was mixed with incoming room air before entering the chamber. Exposure concentrations were determined on both a nominal and actual (gravimetric) basis. Particle size determinations were conducted twice during exposure. During the exposure, control and treated animals were observed every 15 minutes for the first hour and hourly thereafter. On the first day post-exposure, one half of the animals from each group were randomly selected and sacrificed, and an interim necropsy was performed. The remaining animals were observed daily for signs of toxicity for 14 days post-exposure. Body weights were recorded at the beginning of the study, and at 1, 2, 3, 4, 7, and 14 days post-exposure. A necropsy was performed on all animals that died or were sacrificed during the study. Major organs were examined for macroscopic abnormalities and lungs plus trachea, liver, kidneys, whole head, and any abnormal tissues were preserved. Organ weights were recorded at necropsy for lungs plus trachea, liver, and kidneys.

Test substance : CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid)

Conclusion : Under conditions of this study, aerosolized 2,2-Dimethyloctanoic acid has a low order of acute inhalation toxicity in mice, rats, and guinea pigs.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

04.10.2006 (1)

Type : LC50

Value : > 511 mg/m³

Species : guinea pig

Strain : Hartley

Sex : male/female

Number of animals : 20

Vehicle : other: None

Doses :

Exposure time : 6 hour(s)

Method : other

Year : 1982

GLP : no

Test substance :

Remark : No animals died during the study. The control animals appeared normal throughout the exposure. During the two-week post-exposure period, incidences of ungroomed appearance, soft stool, and anogenital staining were observed in some of the control animals. One female guinea pig in the control group died on the fifth day of the post-exposure observation period.

Animals exposed to the test material exhibited some signs of labored breathing, salivation, and eye irritation during the exposure. Upon removal from the chamber, exposed mice and guinea pigs had material-covered fur and exposed rats had some red staining around the nasal area, anogenital staining, soft stool, salivation, and lacrimation. During the two-week post-exposure observation period, all guinea pigs appeared normal. However, some of the mice appeared ungroomed and some rats exhibited anogenital staining and soft stool. Throughout the study, body weights remained normal except for a slight weight loss on the first and second post-exposure days in both the control and treated groups (all species).

At terminal sacrifice, male mice exposed to the aerosolized test substance exhibited a statistically significant decrease in the liver to body weight ratio versus control animals. No other statistically significant differences were

observed for group mean organ weight to body weight ratios. Minor macroscopic abnormalities were observed in both control and treated groups at the interim and terminal necropsies, but were not considered to be related to exposure to the test substance.
Route of administration: Inhalation
Frequency of Treatment: Single 6-hour exposure
Dose/Concentration Levels: Liquid aerosol with a mean analytical concentration of 511 mg/m3
Control group and Treatment: 10/sex/species

Result : LC50 > 511 mg/m3

Test condition : Groups of animals (10/sex/species) were exposed to either air only or to aerosolized test material. Aerosol was generated by pumping the test material into an atomizer at 15.0 psi. The resulting aerosol was sprayed into a glass aerosol diffuser, where it was mixed with incoming room air before entering the chamber. Exposure concentrations were determined on both a nominal and actual (gravimetric) basis. Particle size determinations were conducted twice during exposure. During the exposure, control and treated animals were observed every 15 minutes for the first hour and hourly thereafter. On the first day post-exposure, one half of the animals from each group were randomly selected and sacrificed, and an interim necropsy was performed. The remaining animals were observed daily for signs of toxicity for 14 days post-exposure. Body weights were recorded at the beginning of the study, and at 1, 2, 3, 4, 7, and 14 days post-exposure. A necropsy was performed on all animals that died or were sacrificed during the study. Major organs were examined for macroscopic abnormalities and lungs plus trachea, liver, kidneys, whole head, and any abnormal tissues were preserved. Organ weights were recorded at necropsy for lungs plus trachea, liver, and kidneys.

Test substance : CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid)

Conclusion : Under conditions of this study, aerosolized 2,2-Dimethyloctanoic acid has a low order of acute inhalation toxicity in mice, rats, and guinea pigs.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

04.10.2006 (1)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50

Value : > 3160 mg/kg bw

Species : rabbit

Strain : other: Albino

Sex : male/female

Number of animals : 8

Vehicle : other: None

Doses : 50, 200, 794, 3160 mg/kg

Method : other: NA

Year : 1964

GLP : no

Test substance :

Remark : No deaths occurred with any of the doses tested. The animals appeared normal in appearance and behavior throughout the study. All of the animals exhibited a normal pattern of weight gain. No signs of gross pathology were observed at necropsy.

No dermal irritation was observed at the 50 mg/kg dose level and minimal irritation characterized by slight erythema, atonia, and desquamation that subsided in 10 days was noted at the 200 mg/kg level. At the 794 and 3160 mg/kg levels, a dose-dependent increase in the degree of irritation was observed. This consisted of slight to moderate erythema, which

subsided after the fourth and eighth days, and slight to moderate atonia and desquamation that diminished in severity through the 14-day period.
Route of administration: Dermal
Frequency of Treatment: Single Dose
Dose/Concentration Levels: 50, 200, 794, 3160 mg/kg
Control group and Treatment: None

Result : LD50 > 3160 mg/kg
Test condition : Undiluted test sample was applied to clipped, intact abdominal skin under a dental dam binder. The trunk was subsequently wrapped with gauze and adhesive tape. Following a 24-hour exposure period, binders were removed and the abdominal area was sponged with corn oil to remove sample residue. Following exposure, animals were observed for mortality or toxic effects at 1, 4, and 24 hours, and once daily thereafter for a total of 14 days. A necropsy was performed on any animal that died during the study. At the end of the 14-day observation period, all surviving animals were weighed, sacrificed, and necropsied.
Test substance : CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid)
Conclusion : Under conditions of this study, 2,2-Dimethyloctanoic acid has a low order of acute dermal toxicity in rabbits.
Reliability : (2) valid with restrictions
Study Performed Pre-GLP
Flag : Critical study for SIDS endpoint
16.10.2006 (7)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : undiluted
Exposure : Semiocclusive
Exposure time : 24 hour(s)
Number of animals : 6
Vehicle : other: none
PDII : .67
Result : slightly irritating
Classification :
Method : Directive 92/69/EEC, B.4
Year : 1991
GLP : yes
Test substance :

Method : Approximately 24 hours prior to testing the hair of each animal was clipped on the dorsal surface, from the shoulder region to the lumbar region. The skin was left intact. Elizabethan-type collars were placed around the neck of each rabbit. Only animals with healthy skin were used for the study.

The test substance was administered as a single 0.5 ml dose, introduced under a gauze patch which was secured with tape. The patch was loosely held in contact with the skin by means of a semi-occlusive dressing for the duration of the exposure period. After approximately 4 hours of exposure, the dressing and gauze patch were removed. Residual test substance was removed, where possible, using reverse osmosis water and paper towels without altering existing response or the integrity of the epidermis. Collars were removed after the exposure period.

2 males, and 4 females were tested.

The animals were examined for viability daily. Dermal responses were evaluated approximately 45 minutes, 24, 48, and 72 hours, and 7 days following patch removal. All scoring was made according to the Draize Method of Scoring.

After the Day 7 observation, all animals were sacrificed without further examination.

Result : There were no animal deaths prior to study termination.

Topical application of the test substance elicited very slight erythema in one animal at the 45 minute interval. Erythema increased after the 45 minute interval. At the 24 hour interval, one animal was noted with well-defined erythema and two animals were noted with very slight erythema. At 48 hours, one animal was noted with well-defined erythema, and three animals were noted with very slight erythema. At the 72 hour interval, four animals were noted with very slight erythema. Erythema decreased at the 7 day interval with only one animal noted with very slight erythema.

Edema was not noted during the observation period. Desquamation was noted for three animals at the Day 7 interval.

Based on these finding the primary iiritation index was 0.67, which indicates the test substance is a mild irritant to rabbit skin.

Test substance : CAS No. 26896-20-8; Neodecanoic acid
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
04.10.2006 (2)

Species : rabbit
Concentration :
Exposure : Semiocclusive
Exposure time : 24 hour(s)
Number of animals : 8
Vehicle :
PDII :
Result :
Classification :
Method :
Year : 1964
GLP : no
Test substance :

Remark : No dermal irritation was observed at the 50 mg/kg dose level and minimal irritation characterized by slight erythema, atonia, and desquamation that subsided in 10 days was noted at the 200 mg/kg level. At the 794 and 3160 mg/kg levels, a dose-dependent increase in the degree of irritation was observed. This consisted of slight to moderate erythema, which subsided after the fourth and eighth days, and slight to moderate atonia and desquamation that diminished in severity through the 14-day period.

Route of administration: Dermal
Frequency of Treatment: Single Dose
Dose/Concentration Levels: 50, 200, 794, 3160 mg/kg
Control group and Treatment: None

Test condition : Undiluted test sample was applied to clipped, intact abdominal skin under a dental dam binder. The trunk was subsequently wrapped with gauze and adhesive tape. Following a 24-hour exposure period, binders were removed and the abdominal area was sponged with corn oil to remove sample residue. Following exposure, animals were observed for mortality or toxic effects at 1, 4, and 24 hours, and once daily thereafter for a total of 14 days. A necropsy was performed on any animal that died during the study. At the end of the 14-day observation period, all surviving animals

were weighed, sacrificed, and necropsied.

Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions Study Performed Pre-GLP

16.10.2006 (7)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	undiluted
Dose	:	
Exposure time	:	
Comment	:	not rinsed
Number of animals	:	6
Vehicle	:	none
Result	:	
Classification	:	
Method	:	
Year	:	1964
GLP	:	no
Test substance	:	
Remark	:	Moderate irritation consisting of conjunctivitis, slight transient iritis, and slight corneal opacity was observed. There was some evidence of temporary corneal damage, but the eyes of all animals were completely cleared by the seventh day of observation.
Test condition	:	Animals were individually housed in stainless steel cages, with adequate food and water. The test material was administered as a single instillation of 0.1 ml into the lower conjunctival sac of the left eye of each animal. The upper and lower lids were gently held together for approximately 1 second to prevent loss of the material. The contralateral eye served as the control. The eyes of each animal were examined 24, 48, and 72 hours, and 4, 7 and 10 days after administration. At each interval the treated and control eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Reliability	:	(2) valid with restrictions Study was performed pre-GLP.
Flag	:	Critical study for SIDS endpoint

16.10.2006 (7)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rabbit
Sex	:	male
Strain	:	other: Albino
Route of admin.	:	dermal
Exposure period	:	10 applications with a two-day rest between the 5th and 6th applications.
Frequency of treatm.	:	
Post exposure period	:	
Doses	:	0.4 g/kg and 2.28 g/kg

Control group	:	other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application.
NOAEL	:	= 2280 mg/kg
Method	:	other
Year	:	1964
GLP	:	no
Test substance	:	
Remark	:	Number/sex/dose: 4/dose Vehicle: None Statistical method: Not reported
Result	:	For systemic effects: NOAEL = 2.28 g/kg 2,2-Dimethyloctanoic acid produced moderate skin irritation. Wheezing was noted in one animal of the low dose group. However, the rest of the animals appeared normal in behavior and appearance throughout the study. Animals in the low dose group showed overall body weight gain while animals in the high dose group had a slight reduction in weight at the end of the study. Necropsy revealed parasitic areas on the liver and/or mesentery of three animals, emphysema in three animals, and fluid in the cranial cavity and sinuses of one animal. These findings, however, did not correlate with the dose of test material received and were not attributed to exposure to the test substance. Animals in both the low and high dose groups displayed a decrease in terminal total leukocyte count. However, these values were within the normal limit value for rabbits. Repeat applications did not cause any histopathological alterations to the liver or kidney of the rabbits. Animals in the low dose group displayed slight erythema and moderate atonia and desquamation starting on the first or fourth application and persisting through the remainder of the study. All animals in the high dose group had moderate erythema, moderate to marked atonia and desquamation, and slight edema after the fifth application. After seven applications, slight fissures were observed in some of the animals and the exposed skin became hypersensitive to touch.
Test condition	:	The test material was applied to clipped abdominal skin. A loose gauze binder or a collar was used to prevent ingestion of the test substance. Animals were housed individually and allowed free access to food and water. Each animal was weighed, sacrificed, and necropsied 24 hours after the final application of test material. At the beginning of the study and prior to the final application, the following clinical parameters were evaluated: total erythrocyte count, total and differential leukocyte count, hematocrit, and urinalysis. Histological analysis was performed on sections of liver and kidney. Sections of brain, thyroid, lungs, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved for possible future analysis.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid)
Conclusion	:	Under the conditions of this study, 2,2-Dimethyloctanoic acid has a low order of systemic toxicity following subchronic dermal exposure.
Reliability	:	(2) valid with restrictions Study performed Pre-GLP.
Flag	:	Critical study for SIDS endpoint

04.10.2006 (12)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Bacterial reverse mutation assay
System of testing	:	S. typhimurium TA100, TA1535, TA98, TA1537,
Test concentration	:	
Cycotoxic concentr.	:	

Metabolic activation	:	
Result	:	negative
Method	:	
Year	:	1995
GLP	:	yes
Test substance	:	
Remark	:	Concentrations tested were: 6.17 - 1000 µg/plate without S9. 18.52 - 1500 µg/plate with S9
Result	:	Concentrations up to 1500 µg/plate did not cause a 2-fold or higher increase in the number of revertant colonies of all tested Salmonella strains in the presence or absence of S9 mix after application. Positive controls gave the expected increase in the number of histidine+ revertants in the presence as well as in the absence of S9 mix.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Conclusion	:	Neodecanoic acid is not mutagenic in strains of the bacteria S. typhimurium under conditions of this assay.
Reliability	:	(2) valid with restrictions Although the original data was not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

19.10.2006 (16)

Type	:	Chromosomal aberration test
System of testing	:	Human lymphocytes with and without metabolic activation
Test concentration	:	100 to 800 ug/ml
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	1995
GLP	:	no data
Test substance	:	
Remark	:	Two independent tests were conducted, both in the presence and absence of S9 mix. Cells were exposed to neodecanoic acid for 24 or 48 hours. The cultures were processed for chromosomal aberrations. A mitotic index inhibition was calculated. Concentrations tested: 100 - 400 µg/ml without S9 250 - 800 µg/ml with S9
Result	:	There was no evidence for a statistically significant increase in the % of cells with chromosomal aberrations at each concentration or time point tested, with or without metabolic activation. Positive control substances (mitomycin C and cyclophosphamide) confirmed the activity and sensitivity of the test system.
Test substance	:	CAS No. 26896-20-8; Neodecanoic acid
Conclusion	:	Neodecanoic acid is not genotoxic in human lymphocytes in vitro under conditions of this assay.
Reliability	:	(2) valid with restrictions Although the original data was not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

19.10.2006 (17)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type	:	One generation study
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	other: Dietary
Exposure period	:	
Frequency of treatm.	:	
Premating exposure period		
Male	:	
Female	:	
Duration of test	:	
No. of generation studies	:	
Doses	:	0, 600, 1200, 2500, 5000 ppm in diet
Control group	:	other: 10/sex
Method	:	other
Year	:	1998
GLP	:	yes
Test substance	:	

Remark : No. of animals/sex/dose: 10/sex/dose
Statistics: For the statistical analysis the percent of normal sperm were transformed by Bloom's transformation. All variables were analyzed by standard one-way analysis of variance (ANOVA). Residuals from the model were tested for normality by the Shapiro-Wilk. When there were differences in-group means based on the ANOVA, differences in means were tested using Duncan's multiple range test.
There were no treatment-related deaths or clinical signs noted in the parental animals during this study. There also were no treatment-related clinical signs noted for the offspring. There were no treatment-related effects noted for the male reproductive parameters such as sperm motility, total cauda sperm count, homogenization resistant spermatid count, sperm morphology, or the reproduction indices of mean male fertility, male mating, female fertility, fecundity, or gestational indices. In addition, there were no treatment-related effects on absolute or relative reproductive organ weights.

In the 5000 ppm dose group, statistically significant decreases in parental food consumption were attributed to reduced palatability of the diet. Decreases in body weights were noted in the 5000 ppm females at Gestation Days (GD) 7 and 21 and at Postpartum Days (PPD) 4, 7, and 14. Mean absolute and mean relative liver weights were increased in both sexes of the 5000 ppm group.

The offspring of the 5000 ppm group had reduced Live Birth Index and reduced survival indices on Day 1 and Day 4. Also, offspring body weights of both sexes were reduced during the postnatal period. Offspring body weight was also reduced in males and female of the 2500 ppm group.

Result : Maternal and Offspring NOAEL = 1200 ppm

Test condition : P1 males and females (10 animals/sex) were exposed to the test substance for 10 weeks prior to mating. One male and one female were

paired for up to 2 weeks. Beginning on GD 21, mated females were examined at least twice daily for signs of parturition. On PND 0, 1, 4, 7, 14, 21 and 28 the offspring were counted, sexed and each live pup was weighed. Pups were counted and examined externally on a daily basis during the postnatal period. On PND 4, after counting, weighing, and examining the pups, the size of each litter was adjusted by eliminating extra pups by random selection to yield as nearly as possible, 4 males and 4 females per liter.
Pups from each litter were examined daily for developmental landmarks. Sperm analyses were conducted at necropsy. Surviving F1 females were sacrificed on PND 42 and surviving F1 males were sacrificed on PND 49 unless they had not met criteria for vaginal patency or preputial separation, respectively.

Test substance : Analog substance: Isononanoic Acid (CAS No. 3302-10-1)
Conclusion : Under the conditions of this study the test substance did not adversely affect reproductive parameters at doses that were nontoxic to the dams or their offspring.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
04.10.2006 (10)

Type : other: Three Generation
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : other: Dietary
Exposure period :
Frequency of treatm. : Continuous
Premating exposure period
Male : P1: 9 weeks
Female : P1: 9 weeks
Duration of test : 3 generations
No. of generation studies :
Doses : 0, 100, 500, 1500 ppm in diet
Control group : other: 0, 100, 500, 1500 ppm in diet
NOAEL parental : = 1500 ppm
NOAEL F1 offspring : = 1500 ppm
NOAEL F2 offspring : = 1500 - ppm
Method : other
Year : 1968
GLP : no
Test substance :

Remark : For all of the concentrations tested, no adverse effects were observed on survival, appearance, behavior, body weight gain, and food consumption in either the parental generation or either the F1 or F2 generations. In addition, the reproductive performance of the parents was not affected. No treatment-related gross or microscopic pathological findings were observed at any of the dietary levels.

All of the P1 and P2 animals survived the pre-mating periods and all of the P3 animals survived the 9-week post-weaning period of exposure. The body weight gain, food consumption, appearance, and behavior of the rats in these test groups were comparable with that of the control rats. In the F1A and F1B litters, litter size, pup body weights, appearance, and behavior were comparable between the treated groups and the control group. There were a variety of incidental findings in pups of the F1A and F1B litters, however, pups of these litters did not display any signs of treatment-related toxicity. At necropsy, there were no gross alterations that could be attributed to exposure to the test substance. The F2A and F2B litters, similar to the F1 litters had incidental findings, but did not show any

treatment-related signs of toxicity, or effects on litter size, pup body weights, appearance, or behavior. Examination of the F2B weanling pups also (P3) did not reveal any treatment-related abnormalities.
No. of animals/sex/dose: P1: 80 females and 40 males

Result : NOAEL Parental: 1500 ppm
NOAEL F1 Offspring: 1500 ppm
NOAEL F2 Offspring: 1500 ppm

Test condition : Pre-mating Period: For each dose level, 10 males and 20 females comprised the P1 generation. The parental generation animals were maintained in individual cages and fed the corresponding diet for 9 weeks prior to mating. Individual body weights, food consumption, and observations of the physical appearance and behavior of the animals were recorded initially, at 5 weeks, and 9 weeks (P1), or at 8 weeks, and 12 weeks (P2). The F2B weanlings (P3) were fed the appropriate diets for 9 weeks and the same observations were recorded at 0, 8, and 9 weeks of exposure.

Reproduction Period: Following 9 weeks of exposure, two females and 1 male from each group were housed together and allowed a 3-week mating period, during which time, males were rotated among the females on a weekly basis. 24 hours following birth of the F1A generation, litters were arbitrarily reduced to a maximum of 8 pups (4/sex) to be nursed. The number of conceptions, litters, live births, stillbirths, the size of natural and nursing litters, deaths during the period of lactation, and number of pups weaned were all recorded. The weights of the pups by sex were recorded at 24 hours and at weaning and all pups were observed for gross signs of abnormalities. Following the 21-day nursing period, representative pups from each litter were sacrificed and gross necropsies were performed. The remaining pups were discarded.

One week following the weaning of the F1A litters, the P1 parents were re-mated in the same fashion to produce the F1B pups. Following the 21-day nursing period, 20 female and 10 male weanlings from each of the test groups were randomly designated as the P2 generation. The remaining F1B pups were sacrificed and necropsied. The P2 generation was fed the appropriate diet until 100 days of age and then mated in the same fashion to produce the F2A and F2B litters. The same procedures were followed as during the first reproductive phase. After the second litter, F2B, 20 females and 10 males were selected at random to be the P3 generation. Following 9 weeks of dietary administration to this generation, the study was terminated and gross necropsies were performed. The following tissues were preserved: brain, pituitary, eye, thyroid, lung, heart, liver, spleen, kidney, adrenal, stomach, pancreas, small and large intestine, urinary bladder, gonad, bone, bone marrow, and trachea. Tissues from 5 females and 5 males of the control and high dose groups underwent histological examination. In addition, sections of thyroid, lung, liver, kidney, adrenal and trachea from 5 females and 5 males of the low level and intermediate level groups were examined microscopically.

Test substance : CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid)

Conclusion : Under the conditions of this study, dietary exposure to 2,2-Dimethyloctanoic acid has a low order of reproductive toxicity in rats.

Reliability : (2) valid with restrictions
Study performed pre-GLP

04.10.2006 (13)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Bio/dynamics, Inc. (1982) "Evaluation of the Acute inhalation Toxicity in Rats, Mice, and Guinea Pigs". Unpublished report.

(2) EBSI (1992). Exxon Biomedical Sciences, Inc. Primary Dermal Irritation Study in the Rabbit. Unpublished report.

(3) EG&G Bionomics, Wareham, Mass. BW-78-1-005

(4) EMBSI (2005) Hydrolysis: Neoacids C5 to C28 Category.

(5) EMBSI (2005) Photodegradation (Direct): Neoacids C5 to C28 Category.

(6) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(7) Esso Research and Engineering Company (1964). Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.

(8) Exxon Biomedical Sciences Inc. Ready Biodegradability: OECD 301F Manometric Respirometry Test. 136894A.

(9) Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test. 118358.

(10) Exxon Biomedical Sciences, Inc. (1998) "One generation reproduction toxicity range-finding study in rats," Unpublished report.

(11) ExxonMobil Chemical Company (2003). Neodecanoic acid. Unpublished internal data.

(12) Hazleton Laboratories, Inc. (1964) "Repeated Dermal Application - Rabbits," Unpublished report.

(13) Hazleton Labs, Inc. (1968) "Modified Three-Generation Reproduction Study - Rats," Unpublished report.

(14) Karickoff, S.W., V.K. McDaniel, C. Melton, A.N. Vellino, D.E. Nute, L.A. Carreira (1991). Predicting chemical reactivity by computer. Environ. Toxicol. Chem. 10:1405-1416.

(15) Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model ver. 2.02, available from the Environmental Centre, Trent University, Canada.

(16) TNO (1995). Versatic 10: Bacterial Mutagenic Assay (Ames Test). Unpublished report for Shell.

(17) TNO (1995b). Chromosome Aberration Test in Cultured Human Lymphocytes with Versatic 10. Unpublished report for Shell.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 68938-07-8
CAS No.	:	68938-07-8
EINECS Name	:	Fatty acids, C9-13-neo-
EC No.	:	273-114-3
TSCA Name	:	Fatty acids, C9-13-neo-

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001
Status	:	
Memo	:	ExxonMobil Chemical Company (EMCC) Neoacids - HPV
Printing date	:	06.11.2006
Revision date	:	
Date of last update	:	19.10.2006
Number of pages	:	31
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Neoacids C5 to C28 Category is a group of Neoacids whose physicochemical and toxicological properties are very similar and follow a regular pattern as a result of synthesis and structural similarity. The production of neoacid products involves the reaction between a branched olefin with carbon monoxide and water at elevated temperatures and pressures in the presence of an acid catalyst. The products in this category range in carbon number from C5 to C28.

The six substances share relatively similar physico-chemical properties, which suggests that their environmental fate will be similar. Neoacids are trialkylacetic acids in which each hydrogen on the non carboxyl carbon of acetic acid has been replaced by an alkyl group. There is also a likelihood of common precursors and breakdown products that can result in structurally similar metabolites (e.g. carboxylic acid). Because these substances are similar with regard to environmental behavior/effects and human health, consideration of these substances as a category is justified.

The category also contains propanoic acid, 2,2-dimethyl-, methyl ester (CAS#: 598-98-1). This material is an ester that is rapidly hydrolyzed to the parent neoacid - propanoic acid, 2,2-dimethyl- (CAS#: 75-98-9). Because of this rapid hydrolysis, propanoic acid, 2,2-dimethyl-, methyl ester has properties for health effects, aquatic toxicity, and environmental fate that are consistent with the neoacids.

01.09.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C12H24O2
Molecular weight : 200.32
Petrol class :

Flag : Critical study for SIDS endpoint
04.10.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid

Purity	:	
Colour	:	
Odour	:	
Remark	:	CAS Registry Number, Name, and General Structure for Members of the Neoacids C5 to C28 Category and Analogue Substances: CAS RN: 68938-07-8 TSCA Name: Fatty acids, C9-13-neo- R length (C number): C12 Structure of R: Linear Category Member: Yes

04.10.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

Purity	:	typical for marketed substance
CAS-No	:	68938-07-8
EC-No	:	273-114-3
EINECS-Name	:	Fatty acids, C9-13-neo-
Molecular formula	:	C12H24O2
Value	:	= 99.6 % w/w
Remark	:	The commercial product can be estimated at approximately 87% C9 isomers and approximately 13% C13 isomers, with any remaining isomers within the range indicated.

04.10.2006

1.4 ADDITIVES

Purity type	:	typical for marketed substance
CAS-No	:	68938-07-8
EC-No	:	273-114-3
EINECS-Name	:	Fatty acids, C9-13-neo-
Molecular formula	:	C12H24O2
Value	:	
Function of additive	:	
Remark	:	No additives present

04.10.2006

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Chemical industry: used in synthesis

Remark : Primary use for fatty acids, C9-13, neo- is in the paint and coatings industry.

04.10.2006

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 37 - 76 °C
Sublimation	:	
Method	:	other: ASTM D97
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

12.10.2006 (9)

2.2 BOILING POINT

Value	:	= 236 - 247 °C at
Decomposition	:	
Method	:	other: D1078/01
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

12.10.2006 (9)

2.3 DENSITY

Type	:	
Value	:	= .92 g/cm³ at 20 °C
Method	:	
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

12.10.2006 (9)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .001 - .061 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential vapor pressure for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

12.10.2006 (6)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 3.3 - 5.2 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential partition coefficient for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

12.10.2006 (6)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 3.1 - 243 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	4.8 at 25 °C
Description	:	
Stable	:	
Deg. product	:	

Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	

Method	:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential water solubility for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

12.10.2006 (6)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 124 °C
Type	:	open cup
Method	:	other: COC ASTM D92
Year	:	2003
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

12.10.2006 (9)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	4.8
Method	:	other: calculated

Year	:	2003
GLP	:	
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions The value was calculated based on the chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

12.10.2006 (10)

2.13 VISCOSITY

Value	:	= 53.1 - at 26 °C
Result	:	
Method	:	other: ASTM D445
Year	:	2003
GLP	:	no data
Test substance	:	
Remark	:	Value measured in cSt
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.

12.10.2006 (9)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .000000000000103617 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	

Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (days)	OH- Rate Constant (cm3/molecule-sec)
1.03	10.3617 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C
Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.
Flag : Critical study for SIDS endpoint
12.10.2006 (6)

Type : water
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
Deg. product :
Method : other (calculated): Technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterizing the potential of substances in the Neoacids C5 to C28 Category to undergo direct photodegradation.
Result : Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Neoacids C5 to C28 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References:

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J.

Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Boethling, R.S., Mackay, D. 2000. Handbook of Property Estimation Methods for Chemicals, CRC Press, Boca Raton, FL, USA.

Test substance : Neoacids C5 to C28 Category members
Flag : Critical study for SIDS endpoint
01.09.2006 (5)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method : other: technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterising the potential of substances in the Neoacids C5 to C28 Category to undergo hydrolysis.
Result : Hydrolysis as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

Chemicals that are susecptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances 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). The lack of a suitable leaving group renders a compound resistant to hydrolysis.

Aliphatic acids are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982).

References:

Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

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.

Test substance : Neoacids C5 to C28 Category members
Conclusion : Hydrolysis will not contribute to the removal of neoacids from the

environment.

Flag : Critical study for SIDS endpoint
01.09.2006 (4)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 200.32 g/mol
Water solubility = 123 mg/L (avg of range)
Vapour pressure = 3.10 Pa
log Kow = 4.3
Melting point = 56.5 deg C

Degradation half-lives:

Air - 12.4 hrs
Water - 240000 hrs
Soil - 720000 hrs
Sediment - 7200000 hrs

This model was run assuming 100% discharge to water.

Result :

Air - 0.26%
Water - 41.5%
Soil - 6.6%
Sediment - 51.7%

Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

12.10.2006 (11)

Type	:	fugacity model level I
Media	:	other: air - biota - sediment(s) - soil - water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation according Mackay, Level I
Year	:	2003

Method :

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.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 200.32 g/mol
Water solubility = 123 mg/L (avg of range)
Vapour pressure = 3.10 Pa
log Kow = 4.3
Melting point = 56.5 deg C

Result :

Soil - 87.9%
Air - 5.1%
Water - 5.0%
Sediment - 2.0%
Suspended Sed - 0.06%
Biota - <0.01%

Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Conclusion	:	Results of the Mackay Level I environmental distribution model suggest that Neoacids C5 to C28 Category substances have a potential to partition to soil and air. However, category members are weak organic acids with estimated dissociation constants (pKa) of 4.6 to 4.9 (Karickoff, et. al. 1991). Consequently, category substances at neutral pH, which is typical of most natural surface waters, are expected to dissociate (>99%) to the ionized form and therefore, remain largely in water. The Mackay model is usually limited to non-ionic organics and according to Harris and Hayes, 1982, the ionized species of organic acids are generally adsorbed by soils and sediments to a much lesser degree than are the neutral forms. As a result the Mackay model may overestimate the partitioning of Neoacids C5 to C28 Category substances to the soil and sediment compartments.
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

12.10.2006 (11)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge, domestic
Contact time	:	
Degradation	:	= 2.3 (±) % after 28 day(s)
Result	:	
Deg. product	:	
Method	:	OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year	:	1996
GLP	:	yes
Test substance	:	
Remark	:	Test Type: Manometric Respirometry Test
Result	:	Test material was not readily biodegradable. Half-life was not reached. By day 28, 2.3% degradation of the test material was observed. 10% biodegradation was not achieved by day 28. 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	4.50, 0.00, 2.50	2.33
Na Benzoate	98.9, 95.5	97.2

* replicate data

Test condition	:	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 between 31 and 50 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.
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Conclusion	:	Test substance is considered not readily biodegradable.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

12.10.2006 (7)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF	:	= 3.16
Elimination	:	
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Calculated values using BCFWIN version 2.13, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	BCFWIN estimates the bioconcentration factor (BCF) of an organic compound using the compound's log octanol-water partition coefficient (Kow). The estimation methodology used by BCFWIN is described in "Improved Method for Estimating Bioconcentration Factor (BCF) from Octanol-Water Partition Coefficient", SRC TR-97-006 (2nd Update), July 22, 1997. Log Kow used = 4.89
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential bioaccumulation factor for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

12.10.2006 (6)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 37.5 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	2003
GLP	:	yes
Test substance	:	
Remark	:	Statistical Method: Bionomial Method
Result	:	LC50 = 37.5mg/L (CI 23 to 61), based upon measured concentrations of mean of old and new samples. Analytical method used was GC-FID. LL50 = 38 mg/L (CI 25 to 59), based upon nominal loading levels.

Nominal Conc.	Measured Conc.	% Mortality @ 96 hr.
Control	Below detection	0
6.31 mg/L	5.18 mg/L	0
12.4 mg/L	10.5 mg/L	0
25 mg/L	23 mg/L	0
59 mg/L	61 mg/L	100
104 mg/L	101 mg/L	100

Test condition	:	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 solution was 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 13.7 Deg C. (standard deviation = 0.1 Deg C.), Lighting was 16 hours light : 8 hours dark with 554 to 565 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.3 to 8.7 mg/L and from 5.8 to 6.7 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.3 to 8.0 during the study. Fish were not fed during the study. Fish Mean Wt.= 0.460g. Mean Total length = 4.0cm, Test Loading = 0.535 g of fish/L.
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

12.10.2006 (1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 62.2 measured/nominal
Limit Test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 202
Year	:	2003
GLP	:	yes
Test substance	:	
Remark	:	Statistical Method: Bionomial Method
Result	:	48-hour EC50 = 62.2 mg/L (CI 45.6 - 84.9), based upon measured concentrations of mean of old and new samples. Analytical method used was GC-FID. Nominal Conc. Measured Conc. % Immobilization @ 48 hr. Control 0 0 6.00 mg/L 6.22 mg/L 0 13.5 mg/L 11.5 mg/L 0 26 mg/L 23.5 mg/L 0 52 mg/L 45.6 mg/L 0 102 mg/L 84.9 mg/L 100
Test condition	:	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 via stainless steel and glass syringes. The solutions were mixed for approximately 24 hours at a vortex of </= 10% of the total depth. After mixing, the mixtures were allowed to settle for 1 hour prior to use. 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 20.0 Deg C. (standard deviation = 0.2 Deg C), Lighting was 16 hours light : 8 hours dark with 75.1 to 94.6 Lux during full daylight periods. Dissolved oxygen ranged from 8.2 to 8.4 mg/L during the study. The pH was ranged from 6.7 to 8.2 during the study. Organisms were supplied by in-house cultures. Age = <24 hours old, from 12-day old parents.
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

12.10.2006 (2)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: Pseudokirchneriella subcapitata
Endpoint	:	
Exposure period	:	72 hour(s)
Unit	:	mg/l
NOEC	:	= 226 measured/nominal
EC50	:	= 216 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 201 "Algae, Growth Inhibition Test"

Year : 2003
GLP : yes
Test substance :

Method :

The 72-hour EC50 and EL50 values were determined based on the percent inhibition relative to the control. The specific growth rate for each loading rate/concentration was determined by calculating the slope of the regression line of the ln (cell density) versus time using the PROC REGRESSION procedure from SAS . The areas under the growth curves and average specific growth rate are calculated in accordance with the formulas listed in the OECD guideline2. It was not necessary for this study to have 24 or 48-hour EL50 values (or other statistics) calculated.

The EC50 and EL50 values were calculated by using the inverse interpolation method of Snedecor and Cochran .

The No Observed Effect Loading/Concentration (NOEL/NOEC) values were determined using the ANOVA procedure of SAS.

Result :

72 hour EC50b = 216mg/L (biomass)
72 hour EC50gr = 388mg/L (growth rate)

72 hour NOECRb = 226mg/L (biomass)
72 hour NOECRgr = 226mg/L (growth rate)

Analytical method used was GC-FID.

Nominal Conc. (mg/L)	Mean Cell Growth - 72 hr (% Inhibition)	Conc. - 72 hr (cells/ml)
Control	n/a	1.2 x10E6
64.5 (62.4)*	3.9	1.0 x10E6
125 (120)	4.9	1.0 x10E6
247 (226)	27	3.5 x10E5
531 (350)	51	1.0 x10E5
1054 (432)	59	6.5 x10E4

*note - value in parentheses is mean measured concentration (mg/L)
n/a - Not applicable

Test condition : Individual treatments were prepared for each loading rate by adding the appropriate amount of test substance to algal nutrient media in 2L size glass aspirator bottles. The test substance was added to the aspirator bottles using stainless steel and glass syringes. The syringes were weighed with and without the test substance to determine the actual loading rate. The mixing vessels were sealed with Teflon® covered neoprene stoppers. The mixtures were stirred for 23 hours and 25 minutes on magnetic stirplates with Teflon® coated stirbars at room temperature (22 ± 2°C). The vortex height was set at =10% of the static liquid depth. During mixing, the treatments appeared clear and colorless with the test substance floating on the water surface in the mixing vessels. After mixing, the treatments appeared clear and colorless with the test substance floating on the water surface in the mixing vessels. After stirring, the mixtures were allowed to settle for 1 hour and 5 minutes at 22.0°C before the aqueous portions were removed through the outlet at the bottom of the stirring vessels. The mixtures were adjusted to achieve a pH of 7.4 to 7.6 prior to the filling of the test chambers.

Test chambers were conditioned with the test solutions before the test. Four replicates were prepared for each treatment by filling the test chambers with the WAF. Four replicates of the control were prepared in the same manner using algal nutrient media. Each test flask was

inoculated with ~1.0 x 104 cells per mL. Test cahmbers were 125 ml erlenmeyer flasks with 60 ml of test solution.

Test temperature was 23.8 Deg C. (standard deviation = 0.2 Deg C). Continuous light intensity in the environmental chamber ranged from 8418 to 8804 Lux. Conditions were monitored continuously using a MicroVax 3100-20E running validated custom acquisition software. The oscillation rate was 100 rpm (verified daily).

The pH ranged from 7.5 to 7.6 at test initiation and ranged from 6.6 to 7.0 at termination.

Test substance : CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
12.10.2006 (3)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

Type	:	other: Magnusson-Kligman maximization test
Species	:	guinea pig
Number of animals	:	
Vehicle	:	
Result	:	not sensitizing
Classification	:	
Method	:	
Year	:	1993
GLP	:	no data
Test substance	:	
Remark	:	A Magnusson-Kligman Maximization test showed no indication of sensitization in guinea pigs.
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.

13.10.2006 (14)

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-chronic
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	28 day(s)
Frequency of treatm.	:	1 dose/day
Post exposure period	:	
Doses	:	0, 10, 55, 300 mg/kg/day

Control group	:	other: Polyethylene glycol 200/distilled water (80%/20%) was administered to 10 animals at a level of 1 ml/kg body weight.
NOAEL	:	= 300 - mg/kg bw
Method	:	OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year	:	1994
GLP	:	yes
Test substance	:	
Remark	:	Male and female rats were exposed 5/sex/dose via oral gavage daily for 28 days. Vehicle: Polyethylene glycol 200/distilled water (80%/20%) Control: Polyethylene glycol 200/distilled water (80%/20%) was administered to 10 animals at a level of 1 ml/kg body weight.
Result	:	There were no mortalities. Clinically, increased salivation was observed after dosing in rats receiving 300 mg/kg test substance. No effects on body weight or food consumption were observed. No toxicologically significant changes in hematology parameters, clinical chemistry were observed. In males receiving 300 mg/kg/day, increased kidney weight and abnormal appearance of the kidney at necropsy were noted. Histologically, a dose-related hyaline droplet was noted in males at all treatment levels. The findings in the kidney of the treated males are species and sex specific and are not of toxicological significance for man. No adverse effects were noted in treated females.
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Conclusion	:	Under condition of this study, fatty acids, C9-C13 neo does not cause significant toxic effects after repeated exposure.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

13.10.2006 (12)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Bacterial reverse mutation assay
System of testing	:	Ames Salmonella assay with and without metabolic activation and E.coli
Test concentration	:	31.25 to 5000 ug/plate
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471
Year	:	1993
GLP	:	yes
Test substance	:	
Result	:	There was no increase in reverse mutation rate in either the presence or absence of S9. No evidence of cytotoxcity was observed in these assays at any of the concentrations tested. The control substances demonstrated system activity and sensitivity.
Test condition	:	Species/strain tested: S. typhimurium TA 1535, 1537, 98, 100 and E. coli WP2uvrA pKM101 Species/cell type: Rat liver (S9) fraction Concentrations tested: 31.25 - 5000 µg/plate ± S9. All diluted in acetone. Solubility of test substance was limited at concentrations of 2000 - 5000 µg/plate.

Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Conclusion	:	Fatty acids, C9-C13 neo is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay.
Reliability	:	(2) valid with restrictions Although the original data was not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

19.10.2006 (13)

Type	:	Chromosomal aberration test
System of testing	:	Chinese Hamster Ovary (CHO) cells
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	
Method	:	
Year	:	1994
GLP	:	yes
Test substance	:	

Result : In the absence of rat liver S9, mitotic inhibition was 62% at 218.75 µg/ml and in a second experiment 62% at 250 µg/ml. In the presence of S9, no cytotoxicity was noted at 800 µg/ml and in a second experiment 79% mitotic inhibition at 1000 µg/ml with insufficient scorable metaphases. In the absence of S9 there were no increases in structural chromosome damage upon exposure of cultures up to toxic concentrations for 48 hours. In the presence of S9, the number of cells with structural chromosomal aberrations (excluding as well as including gaps, isogaps) were statistically increased at concentrations of 400 above upon exposure for 24 and 48 hours. The control substances demonstrated system activity and sensitivity.

Test condition : System tested: Chinese hamster ovary cells (CHO-K1) with and without metabolic activation

Species/cell type: Rat liver (S9) fraction

Dose levels -S9 (µg/ml)

24-hrs: 0, 13.67, 109.38, 218.75
0, 25, 125, 250

48-hrs: 0, 125

Dose levels +S9 (µg/ml)

24-hrs: 0, 100, 400, 800
0, 100, 400, 1000

48-hrs: 0, 750

Dose selection was based on a preliminary study covering doses of 3.42 to 1750 µg/ml (solubility limit in the medium).

Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Conclusion	:	Fatty acids, C9-C13 neo induces chromosomal aberrations in CHO cells in the presence of S9; however, no chromosomal aberration was observed in the absence of S9.
Reliability	:	(2) valid with restrictions Although the original data was not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

19.10.2006 (15)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	other: Micronucleus test in vivo
Species	:	mouse
Sex	:	male/female
Strain	:	other: Swiss (Charles River CD-1)
Route of admin.	:	other: oral gavage
Exposure period	:	
Doses	:	0, 2000 mg/kg (limit dose); diluted in PEG 200/water (80/20 w/w)
Result	:	negative
Method	:	
Year	:	1995
GLP	:	yes
Test substance	:	other TS: Fatty acids, C9-13-neo- (CAS No. 68938-07-8)
Result	:	No differences were observed in frequencies of micronucleated polychromatic erythrocytes (MPE) per 1000 polychromatic erythrocytes (PE) and PE per 1000 al associated mature erythrocytes.
Test condition	:	Number: 10/sex/dose Frequency: Single dose At 24 and 48 hours after dosing, 5 males and 5 females were sacrificed. Bone marrow was collected and processed into two bone marrow smears for each animal. Methanol was used for fixation of smears, which were stained with May-Grunwald Giemsa and microscopically examined.
Test substance	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo-
Conclusion	:	Fatty acids, C9-C13 neo did not induce cytogenetic damage to the bone marrow of Swiss mice under these conditions.
Reliability	:	(2) valid with restrictions Although the original data was not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

19.10.2006 (16)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type	:	other: One generation study
In vitro/in vivo	:	In vivo
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	for 10 weeks prior to mating
Frequency of treatm.	:	daily

Duration of test	:	One generation
Doses	:	0, 600, 1200, 2500, 5000 ppm in diet
Control group	:	yes
Method	:	
Year	:	1998
GLP	:	yes
Test substance	:	

Remark : For the statistical analysis the percent of normal sperm were transformed by Bloom's transformation. All variables were analyzed by standard one-way analysis of variance (ANOVA). Residuals from the model were tested for normality by the Shapiro-Wilk. When there were differences in-group means based on the ANOVA, differences in means were tested using Duncan's multiple range test.
There were no treatment-related deaths or clinical signs noted in the parental animals during this study. There also were no treatment-related clinical signs noted for the offspring. There were no treatment-related effects noted for the male reproductive parameters such as sperm motility, total cauda sperm count, homogenization resistant spermatid count, sperm morphology, or the reproduction indices of mean male fertility, male mating, female fertility, fecundity, or gestational indices. In addition, there were no treatment-related effects on absolute or relative reproductive organ weights.

In the 5000 ppm dose group, statistically significant decreases in parental food consumption were attributed to reduced palatability of the diet. Decreases in body weights were noted in the 5000 ppm females at Gestation Days (GD) 7 and 21 and at Postpartum Days (PPD) 4, 7, and 14. Mean absolute and mean relative liver weights were increased in both sexes of the 5000 ppm group.

The offspring of the 5000 ppm group had reduced Live Birth Index and reduced survival indices on Day 1 and Day 4. Also, offspring body weights of both sexes were reduced during the postnatal period. Offspring body weight was also reduced in males and female of the 2500 ppm group.

Result :

Maternal and Offspring NOAEL = 1200 ppm

Test condition : Test material was assumed to be 100% pure for purposes of dosing. P1 males and females (10 animals/sex) were exposed to the test substance for 10 weeks prior to mating. One male and one female were paired for up to 2 weeks. Beginning on GD 21, mated females were examined at least twice daily for signs of parturition. On PND 0, 1, 4, 7, 14, 21 and 28 the offspring were counted, sexed and each live pup was weighed. Pups were counted and examined externally on a daily basis during the postnatal period. On PND 4, after counting, weighing, and examining the pups, the size of each litter was adjusted by eliminating extra pups by random selection to yield as nearly as possible, 4 males and 4 females per liter. Pups from each litter were examined daily for developmental landmarks. Sperm analyses were conducted at necropsy. Surviving F1 females were sacrificed on PND 42 and surviving F1 males were sacrificed on PND 49 unless they had not met criteria for vaginal patency or preputial separation, respectively.

Test substance : Analog material: CAS No. 3302-10-1; Isononanoic acid

Conclusion : Under the conditions of this study the test substance did not adversely affect reproductive parameters at doses that were nontoxic to the dams or their offspring.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

13.10.2006 (8)

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) EMBSI (2003b). ExxonMobil Biomedical Sciences, Inc. Fish, Acute Toxicity Test. Study No. 145658. Unpublished report.

(2) EMBSI (2003c). ExxonMobil Biomedical Sciences, Inc. Daphnia sp., Acute Immobilization Test. Study No. 145642A. Unpublished report.

(3) EMBSI (2003d). ExxonMobil Biomedical Sciences, Inc. Alga, Growth Inhibition Test. Study No. 145667. Unpublished report.

(4) EMBSI (2005) Hydrolysis: Neoacids C5 to C28 Category.

(5) EMBSI (2005) Photodegradation (Direct): Neoacids C5 to C28 Category.

(6) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(7) Exxon Biomedical Sciences Inc. Ready Biodegradability: OECD 301F Manometric Respirometry Test. 136894A.

(8) Exxon Biomedical Sciences, Inc. (1998) "One generation reproduction toxicity range-finding study in rats," Unpublished report.

(9) ExxonMobil Chemical Company (2003). Fatty acids, C9-13-neo. Unpublished internal data.

(10) Karickoff, S.W., V.K. McDaniel, C. Melton, A.N. Vellino, D.E. Nute, L.A. Carreira (1991). Predicting chemical reactivity by computer. Environ. Toxicol. Chem. 10:1405-1416.

(11) Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model ver. 2.02, available from the Environmental Centre, Trent University, Canada.

(12) Shell International Petroleum Maatschappij. (1994) "28-day oral (gavage administration) sub-chronic toxicity study in the rat.

(13) Shell Research Ltd. (1993). Versatic 913D: Bacterial Mutagenicity Studies. Unpublished report.

(14) Shell Research Ltd. (1993a). Acute Oral and Dermal Toxicity in Rat, Skin and Eye Irritancy in Rabbit and Skin Sensitizing Potential in guinea pigs. Unpublished report.

(15) Shell Research Ltd., (1993). Versatic 913D: In Vitro Chromosome Studies Using Chinese Hamster Ovary (CHO) Cells. Unpublished report.

(16) TNO (1995). Assessment of Versatic 913D for mutagenic activity in vivo in a micronucleus test in mice. Unpublished report for Shell.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 72480-45-6
CAS No.	:	72480-45-6
TSCA Name	:	Fatty acids, C9-28-neo-
Molecular Formula	:	Unspecified
Producer related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001
Substance related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001
Status	:	
Memo	:	ExxonMobil Chemical Company (EMCC) Neoacids - HPV
Printing date	:	06.11.2006
Revision date	:	
Date of last update	:	16.10.2006
Number of pages	:	23
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Neoacids C5 to C28 Category is a group of Neoacids whose physicochemical and toxicological properties are very similar and follow a regular pattern as a result of synthesis and structural similarity. The production of neoacid products involves the reaction between a branched olefin with carbon monoxide and water at elevated temperatures and pressures in the presence of an acid catalyst. The products in this category range in carbon number from C5 to C28.

The six substances share relatively similar physico-chemical properties, which suggests that their environmental fate will be similar. Neoacids are trialkylacetic acids in which each hydrogen on the non carboxyl carbon of acetic acid has been replaced by an alkyl group. There is also a likelihood of common precursors and breakdown products that can result in structurally similar metabolites (e.g. carboxylic acid). Because these substances are similar with regard to environmental behavior/effects and human health, consideration of these substances as a category is justified.

The category also contains propanoic acid, 2,2-dimethyl-, methyl ester (CAS#: 598-98-1). This material is an ester that is rapidly hydrolyzed to the parent neoacid - propanoic acid, 2,2-dimethyl- (CAS#: 75-98-9). Because of this rapid hydrolysis, propanoic acid, 2,2-dimethyl-, methyl ester has properties for health effects, aquatic toxicity, and environmental fate that are consistent with the neoacids.

01.09.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C19H38O2
Molecular weight : 298.51
Petrol class :

Flag : Critical study for SIDS endpoint
13.10.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid

Purity	:	
Colour	:	
Odour	:	
Remark	:	CAS Registry Number, Name, and General Structure for Members of the Neoacids C5 to C28 Category and Analogue Substances: CAS RN: 72480-45-6 TSCA Name: Fatty acids, C9-28-neo- R length (C number): C19 Structure of R: Linear Category Member: Yes

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1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

Purity	:	typical for marketed substance
CAS-No	:	72480-45-6
EC-No	:	
EINECS-Name	:	Fatty acids, C9-28-neo-
Molecular formula	:	C19H38O2
Value	:	= 99.6 % w/w
Remark	:	The commercial product is a complex combination of fatty acids obtained by the hydolysis of boron trifluoride esters of neoacids produced by the carboxylation and polymerization of isobutylene and nonene. It consists primarily of fatty acids having carbon numbers predominantly in the range of C9 through C28 and boiling in the range of approximately 225 to 387°C.

13.10.2006

1.4 ADDITIVES

Purity type	:	typical for marketed substance
CAS-No	:	72480-45-6
EC-No	:	
EINECS-Name	:	Fatty acids, C9-28-neo-
Molecular formula	:	C19H38O2
Value	:	
Function of additive	:	
Remark	:	No additives present

13.10.2006

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Chemical industry: used in synthesis
Remark	:	Primary use for fatty acids, C9-28, neo- is in the paint and coatings industry.

13.10.2006

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 37 - 76 °C
Sublimation	:	
Method	:	other: ASTM D97
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 72480-45-6; Fatty acids, C9-28-neo-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

16.10.2006 (4)

2.2 BOILING POINT

Value	:	= 236 - 247 °C at
Decomposition	:	
Method	:	other: D1078/01
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 72480-45-6; Fatty acids, C9-28-neo-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

16.10.2006 (4)

2.3 DENSITY

Type	:	density
Value	:	= .92 g/cm³ at 20 °C
Method	:	
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 72480-45-6; Fatty acids, C9-28-neo-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

16.10.2006 (4)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .0000000000023 - .061 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 72480-45-6; Fatty acids, C9-28-neo-
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential vapor pressure for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

16.10.2006 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 3.3 - 6 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Calculated values using KOWWIN versio. 1.65, a su broutine of the computer program EPIWIN version 3.04
Test condition	:	Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	CAS No. 72480-45-6; Fatty acids, C9-28-neo-
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential vapor pressure for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

16.10.2006 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	< 1 - 243 at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	4.9 at 25 °C
Description	:	
Stable	:	
Deg. product	:	

Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	

Method	:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 72480-45-6; Fatty acids, C9-28-neo-
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential vapor pressure for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

16.10.2006 (3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 118.3 °C
Type	:	closed cup
Method	:	other: PMCC ASTM D93
Year	:	2003
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 72480-45-6; Fatty acids, C9-28-neo-
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

16.10.2006 (4)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	4.9
Method	:	other: calculated

Year	:	2003
GLP	:	
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 72480-45-6; Fatty acids, C9-28-neo-
Reliability	:	(2) valid with restrictions The value was calculated based on the chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

16.10.2006 (5)

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .000000000000202531 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year	:	2003
GLP	:	
Test substance	:	

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (days)	OH- Rate Constant (cm3/molecule-sec)
0.53	20.2531 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C

Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : CAS No. 72480-45-6; Fatty acids, C9-28-neo-

Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.

Flag : Critical study for SIDS endpoint
16.10.2006 (3)

Type : water
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
Deg. product :
Method : other (calculated): Technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterizing the potential of substances in the Neoacids C5 to C28 Category to undergo direct photodegradation.

Result : Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Neoacids C5 to C28 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References:

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Boethling, R.S., Mackay, D. 2000. Handbook of Property Estimation Methods for Chemicals, CRC Press, Boca Raton, FL, USA.

Test substance : Neoacids C5 to C28 Category members
Flag : Critical study for SIDS endpoint
01.09.2006 (2)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method : other: technical discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterising the potential of substances in the Neoacids C5 to C28 Category to undergo hydrolysis.
Result : Hydrolysis as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

Chemicals that are susecptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances 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). The lack of a suitable leaving group renders a compound resistant to hydrolysis.

Aliphatic acids are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982).

References:

Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

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.

Test substance : Neoacids C5 to C28 Category members
Conclusion : Hydrolysis will not contribute to the removal of neoacids from the environment.

Flag : Critical study for SIDS endpoint
01.09.2006 (1)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 298.51 g/mol
Water solubility = 65 mg/L (avg of range)
Vapour pressure = 0.10 Pa
log Kow = 4.7
Melting point = 56.5 deg C

Degradation half-lives:

Air - 12.4 hrs
Water - 240000 hrs
Soil - 720000 hrs
Sediment - 7200000 hrs

This model was run assuming 100% discharge to water.

Result :

Air - 0.01%
Water - 20.3%
Soil - 10.2%
Sediment - 69.5%

Test substance : CAS No. 72480-45-6; Fatty acids, C9-28-neo-

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
16.10.2006 (6)

Type : fugacity model level I
Media : other: air - biota - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level I
Year : 2003

Method : 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.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 298.51 g/mol
Water solubility = 65 mg/L (avg of range)
Vapour pressure = 0.10 Pa
log Kow = 4.7
Melting point = 56.5 deg C

Result :

Soil - 95.5%
Air - 0.2%
Water - 2.1%
Sediment - 2.1%
Suspended Sed - 0.07%
Biota - <0.01%

Test substance : CAS No. 72480-45-6; Fatty acids, C9-28-neo-
Conclusion : Results of the Mackay Level I environmental distribution model suggest that Neoacids C5 to C28 Category substances have a potential to partition to soil and air. However, category members are weak organic acids with estimated dissociation constants (pKa) of 4.6 to 4.9 (Karickoff, et. al. 1991). Consequently, category substances at neutral pH, which is typical of most natural surface waters, are expected to dissociate (>99%) to the ionized form and therefore, remain largely in water.

The Mackay model is usually limited to non-ionic organics and according to Harris and Hayes, 1982, the ionized species of organic acids are generally adsorbed by soils and sediments to a much lesser degree than are the neutral forms. As a result the Mackay model may overestimate the partitioning of Neoacids C5 to C28 Category substances to the soil and sediment compartments.

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
16.10.2006 (6)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum :

Remark : No data are available
16.10.2006

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF : = 3.16 -
Elimination :
Method : other: calculated
Year : 2003
GLP :
Test substance :

Method : Calculated values using BCFWIN version 2.13, a subroutine of the computer program EPIWIN version 3.04
Test condition : BCFWIN estimates the bioconcentration factor (BCF) of an organic compound using the compound's log octanol-water partition coefficient (Kow).

The estimation methodology used by BCFWIN is described in "Improved Method for Estimating Bioconcentration Factor (BCF) from Octanol-Water Partition Coefficient", SRC TR-97-006 (2nd Update), July 22, 1997.

Log Kow used = 4.7
Test substance : CAS No. 72480-45-6; Fatty acids, C9-28-neo-
Reliability : (2) valid with restrictions
The result is a calculated value based on the chemical structure and represents a potential bioaccumulation factor for the substance with the CAS number listed under test substance.
Flag : Critical study for SIDS endpoint
16.10.2006 (3)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) EMBSI (2005) Hydrolysis: Neoacids C5 to C28 Category.

(2) EMBSI (2005) Photodegradation (Direct): Neoacids C5 to C28 Category.

(3) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(4) ExxonMobil Chemical Company (2003). Fatty acids, C9-28-neo. Unpublished internal data.

(5) Karickoff, S.W., V.K. McDaniel, C. Melton, A.N. Vellino, D.E. Nute, L.A. Carreira (1991). Predicting chemical reactivity by computer. Environ. Toxicol. Chem. 10:1405-1416.

(6) Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model ver. 2.02, available from the Environmental Centre, Trent University, Canada.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT