IUCLID



Data Set

-

Existing Chemical CAS No. EINECS Name EC No. TSCA Name Molecular Formula	 ID: 598-98-1 598-98-1 methyl pivalate 209-959-1 Propanoic acid, 2,2-dimethyl-, methyl ester C6H12O2
Producer related part Company Creation date	: ExxonMobil Biomedical Sciences Inc. : 18.09.2001
Substance related part Company Creation date	: ExxonMobil Biomedical Sciences Inc. : 18.09.2001
Status Memo	: ExxonMobil Chemical Company (EMCC) Neoacids - HPV
Printing date Revision date	: 06.11.2006
Date of last update	: 16.10.2006 · 23
Chapter (profile) Reliability (profile) Flags (profile)	 Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 Reliability: without reliability, 1, 2, 3, 4 Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

ld 598-98-1 Date 06.11.2006

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

erre	эе	text
2	ee tre	e tree

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 Neoacids are trialkylacetic acids in which each hydrogen on the non carboxyl carbon of acetic acid has been replaced by an alkyl group.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 Molecular weight Petrol class	:	C6H12O2 116.16
Flag 21.09.2006	:	Critical study for SIDS endpoint

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid

1. General Informa	tion	Date 06.11 2006
		24.0 00.11.2000
Purity Colour Odour	: : :	
Remark	: CAS Registry Number, Name, and General Struct Neoacids C5 to C28 Category and Analogue Subs	ture for Members of the stances:
	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 1	FRADENAMES	
methyl pivalate		
11.11.2004		
1.3 IMPURITIES		
Purity CAS-No	: typical for marketed substance : 598-98-1	
EC-No	: 209-959-1	
EINECS-Name Molecular formula	: methyl pivalate : C6H12O2	
Value	: = 99 % w/w	
21.09.2006		
Purity type	: typical for marketed substance	
CAS-No	:	
EC-NO EINECS-Name		
Molecular formula	:	
Value Function of additive		
	- 	
Remark 21.09.2006	: No additives present.	
1.5 TOTAL QUANTITY		
I.U.I LADELLING		

Г

1. General Information	ld 598-98-1 Date 06.11.2006
1.6.2 CLASSIFICATION	
1.6.3 PACKAGING	
1.7 USE PATTERN	
Type of use: industrialCategory: Chemical industry: use	d in synthesis
Remark: Primarily used as a cor21.09.2006	nponent in the production of vinyl chloride resins.
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 PRODUC	стя
1.9.2 COMPONENTS	
1.10 SOURCE OF EXPOSURE	

1. G	eneral Information	ld Date	598-98-1 06.11.2006
1.11	ADDITIONAL REMARKS		
1.12	LAST LITERATURE SEARCH		
1.13	REVIEWS		

2.1 MELTING POINT

Value Sublimation Method Year GLP Test substance	: = -62.5 °C : other: calculated : 2003	
Method Test condition	 Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04 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.	
Test substance Reliability	 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. CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester (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 	r
Flag 21.09.2006	: Critical study for SIDS endpoint (3)
2.2 BOILING POINT		
Value Decomposition Method Year GLP Test substance	: = 101 °C at 1013 hPa : : other: D1078/01 : 2003 : no data :	
Test substance Reliability Flag	 CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester (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. Critical study for SIDS endpoint 	`
18.10.2006	(4)
2.3 DENSITY		
Type Value Method Year GLP Test substance	 density = .87 g/cm³ at 20 °C other: ASTM D4052/86 equivalent 2003 no data 	

2. Physico-Chemi	cal Data	ld 598-98-1 Date 06.11.2006
Test substance Reliability	 CAS No. 598-98-1; Propanoic acid, 2,2- (2) valid with restrictions Although the original data were not retriver were developed following acceptable technological considered reliable. 	dimethyl-, methyl ester eved and reviewed for quality, they st methods and therefore
Flag 21.09.2006	: Critical study for SIDS endpoint	(4
2.3.1 GRANULOMETRY	(
2.4 VAPOUR PRESS	JRE	
Value Decomposition Method Year GLP Test substance	 = 47.6 hPa at 25 °C other (calculated) 2003 	
Method Remark	 Vapor pressure calculation by MPBPWI method of Grain. EPIWIN is used and advocated by the L 	N ver. 1.40 using calculation JS EPA for chemical property
Test substance Reliability	 estimation. CAS No. 598-98-1; Propanoic acid, 2,2- (2) valid with restrictions The result is a calculated value based o represents a potential vapor pressure for number listed under test substance. 	dimethyl-, methyl ester on the chemical structure and or the substance with the CAS
Flag 21.09.2006	: Critical study for SIDS endpoint	(5
2.5 PARTITION COEF	FICIENT	
Partition coefficient Log pow pH value Method Year GLP Test substance	 octanol-water = 1.8 at 25 °C other (calculated) 2003 : 	
Remark Test substance Reliability	 Value was provided by the experimenta CAS No. 598-98-1; Propanoic acid, 2,2- (2) valid with restrictions Although the original data were not retriver were developed following acceptable teconsidered reliable. 	I database of the EPIWIN program dimethyl-, methyl ester eved and reviewed for quality, the st methods and therefore

(3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Flag

21.09.2006

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

: Critical study for SIDS endpoint

2. Physico-Chemical Data

Id 598-98-1 Date 06.11.2006

concentration		at °C	
Temperature effects	:		
Examina different nol	:		
Examine different pol.	:		
pra Description		4.0 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)

(3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value Type Method Year GLP Test substance	: = 7 °C : closed cup : other: TCC ASTM D56 : 2003 :
Test substance Reliability	 CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester (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 21.09.2006	: Critical study for SIDS endpoint (4)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2. Physico-Chemical Data

ld 598-98-1 Date 06.11.2006

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant Method Year GLP Test substance		4.6 other: calculated 2003
Method Remark	:	pKa calculation by SPARC 2003 using a Linux Calculation engine. SPARC On-line calculator can be accessed at
Test substance Reliability	:	 http://ibmlc2.chem.uga.edu/sparc/index.cfm CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester (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 Result Method Year GLP Test substance	 = 1 - at 25 °C other: ASTM D445 2003 no data 	
Remark Test substance Reliability	 Value measured in cSt CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester (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. 	1
21.09.2006	(4	1)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type Light source Light spectrum Relative intensity INDIRECT PHOTOLYSIS Sensitizer Conc. of sensitizer Rate constant Degradation Deg. product Method Year GLP Test substance		air Sun light nm based on intensity of OH 1500000 molecule/cm = .000000000007194 % after other (calculated): Ca subroutine of the comp 2003	of sunlight ³ 4 cm³/(molecule*sec) Ilculated values using AOPWIN version 1.89, a puter program EPIWIN version 3.04
Result	•	Atmospheric Oxidation	n Potential
in the sum	•	In the environment, or degraded by several in transformation proces hydroxyl (OH-) radical organic compound rea atmospheric persisten	ganic chemicals emitted into the troposphere are mportant transformation processes. The dominant s for most compounds is the daylight reaction with s (Atkinson, 1988, 1989). The rate at which an acts with OH- radicals is a direct measure of its ce (Meylan and Howard, 1993).
		AOPWIN estimates th reaction between phot chemicals. The rate c calculate atmospheric average atmospheric	e rate constant for the atmospheric, gas-phase tochemically produced hydroxyl radicals and organic constants estimated by the program are then used to half-lives for organic compounds based upon concentrations of hydroxyl radicals.
		Since the reactions or atmospheric half-lives	ly take place in the presence of sunlight, the 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. Est for organic chemicals.	timation of gas-phase hydroxyl radical rate constants Environ. Toxicol. Chem. 7:435-442.
		Atkinson, R. 1989. Kir the hydroxyl radical wi Monograph No. 1, Am	netics and mechanisms of the gas-phase reactions of ith organic compounds. J. Phys. Chem. Ref. Data er. Inst. Physics & Amer. Chem. Soc., NY.
Test condition	:	Meylan, W.M. and P.H atmospheric gas-phas radicals and ozone. C Indirect photodegrada the structure-activity re	H. Howard. 1993. Computer estimation of the se reaction rate of organic compounds with hydroxyl hemosphere 12:2293-2299. tion, or atmospheric oxidation potential, is based on elationship methods developed by R. Atkinson.
		Temperature: 25°C	
		10 /	23

Id 598-98-1

Date 06.11.2006

Test substance Reliability	 Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3 CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester (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 21.09.2006	: Critical study for SIDS endpoint (3)
Type Light source Light spectrum Relative intensity Deg. product Method Year GLP Test substance	water nm based on intensity of sunlight other (calculated): Technical discussion
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 the event the phone to the produce.
	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
	11/23

3. Environmenta	Fate and Pathways	ld 598-98-1 Date 06.11.2006
	Property Estimation Methods, McGraw-I USA.	Hill Book Company, New York,
	Zepp, R. G. and D. M. Cline. 1977. Rate Aqueous Environment, Environ. Sci. Teo	es of Direct Photolysis in the chnol., 11:359-366.
Test substance Flag	 Boethling, R.S., Mackay, D. 2000. Hand Methods for Chemicals, CRC Press, Bo Neoacids C5 to C28 Category members Critical study for SIDS endpoint 	dbook of Property Estimation ca Raton, FL, USA. s
01.09.2006		(2)
3.1.2 STABILITY IN W	ATER	
Type t1/2 pH4 t1/2 pH7 t1/2 pH9 Deg. product Method Year GLP Tost substance	abiotic at °C at °C at °C at °C other: technical discussion	
Remark	·	prostariaing the natential of
Result	substances in the Neoacids C5 to C28 (Hydrolysis as a Function of Molecular S	Category to undergo hydrolysis.
	Hydrolysis of an organic molecule occur with water (H2O) to form a new carbon- bond is cleaved (Gould, 1959; Harris, 19 is referred to as a nucleophilic substitution group being replaced by the incoming ne molecule.	rs when a molecule (R-X) reacts oxygen bond after the carbon-X 982). Mechanistically, this reaction on reaction, where X is the leaving ucleophilic oxygen from the water
	Chemicals that are susecptible to hydro can be displaced by a nucleophilic subs have a potential to hydrolyze include alk carboxylic acid esters and lactones, epo sulfonic acid esters (Neely, 1985). The I renders a compound resistant to hydroly	lysis contain functional groups that titution reaction. Substances that kyl halides, amides, carbamates, oxides, phosphate esters, and ack of a suitable leaving group ysis.
	Aliphatic acids are resistant to hydrolysis group that is hydrolytically reactive (Har	s because they lack a functional ris, 1982).
	References:	
	Gould, E.S. (1959), Mechanism and Stru Reinhart and Winston, New York, NY, U	ucture in Organic Chemistry, Holt, JSA.
	Harris, J.C. (1982), "Rate of Hydrolysis," Reehl, and D.H. Rosenblatt, eds., Hand Estimation Methods, McGraw-Hill Book	" Chapter 7 in: W.J. Lyman, W.F. book of Chemical Property Company, New York, NY, USA.
Test substance Conclusion	 Neely, W. B. 1985. Hydrolysis. In: W. B. Environmental Exposure from Chemical Boca Raton, FL, USA. Neoacids C5 to C28 Category members Hydrolysis will not contribute to the removement 	Neely and G. E. Blau, eds. ls. Vol I., pp. 157-173. CRC Press, s oval of neoacids from the

3. Environmental Fa	te and Pathways	ld Date	598-98-1 06.11.2006
Flag 01.09.2006	: Critical study for SIDS endpoint		(1)
3.1.3 STABILITY IN SOIL			
3.2.1 MONITORING DATA			
3.2.2 FIELD STUDIES			
3.3.1 TRANSPORT BETW	EEN ENVIRONMENTAL COMPARTMENTS		
Type Media Air Water Soil Biota Soil Method YearMethod Year	 fugacity model level III other: air - sediment(s) - soil - water % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I)/III) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) other: Calculation according Mackay, Level I 2003 The EQC Level III model is a steady state m determining how the medium of release affe III fugacity allows non-equilibrium conditions media as steady state, and illustrate importa processes. Physicochemical input values for the model EPIWIN Estimation v 3.04 program. Measu used where available and obtained from the data from the equilibrium model provide bas partitioning behavior of chemicals between s compartments (i.e., air, water, soil, and sedii 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 This model was run assuming 100% dischart Air - 13.7% Water - 86.0% Soil - 0.03% 	III nodel that is cts environ to exist be int transpor were calcu red input va EPIWIN da ic informati selected en ment).	s useful for mental fate. Level tween connected t and transformation lated using the alues were also atabase. Distribution on on the potential vironmental
Test substance	Sediment - 0.28% CAS No. 598-98-1; Propanoic acid, 2,2-dime	ethyl-, meth	nyl ester
	13 / 23		

ld 598-98-1 Date 06.11.2006

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 Media Air Water Soil Biota Soil Method Year		fugacity model level I other: air - biota - sediment(s) - soil - water % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) other: Calculation according Mackay, Level I 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:
Result		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
	•	Soil - 0.1% Air - 97.1% Water - 2.5% Sediment - <0.01% Suspended Sed - <0.01% Biota - <0.01%
Test substance Conclusion	:	CAS No. 598-98-1; Propanoic acid, 2,2-dimethyl-, methyl ester 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.
Deliebility	_	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.
Keliability	:	(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 2 Method other: calculated 2 Year 2003 2 GLP 2 Test substance 2 Method : Calculated values using BCFWIN version 2.13, a subroutine of the computer program EPIWIN version 3.04 BCFWIN estimates the bioconcentration factor (BCF) of an organic **Test condition** : 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 = 1.83Test 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. : Critical study for SIDS endpoint Flag 22.09.2006 (3)

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

ld 598-98-1 Date 06.11.2006

- 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. To	xicity	ld Date	598-98-1 06.11.2006
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. Toxicity

ld 598-98-1 Date 06.11.2006

5.11 ADDITIONAL REMARKS

6. Analyt. Meth. for Detection and Identification	
---	--

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses Id 598-98-1						
	Da	e	06.11.2006			
7.1	FUNCTION					
7.2	EFFECTS ON ORGANISMS TO BE CONTROLLED					
7.3	ORGANISMS TO BE PROTECTED					
7.4	USER					
7.5	RESISTANCE					

8.	Meas.	Nec.	to Prot.	Man,	Animals,	Environment
----	-------	------	----------	------	----------	-------------

- 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

9. References

- (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

RECEIVED OPPT CBIC 2006 NOV 14 AM 9: 22

í .

IUCLID

Data Set

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

ld 75-98-9 Date 06.11.2006

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

erre	эе	text
2	ee tre	e tree

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 Molecular weight Petrol class	::	C5H10O2 102.13
Flag 01.09.2006	:	Critical study for SIDS endpoint

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid

I. General Info	ormation	ld 75-98-9 Date 06.11.2006
Purity Colour Odour		
Remark	: CAS Registry Number, Name Neoacids C5 to C28 Category	, and General Structure for Members of the / 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 substanc	е
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	:	

1. General Informat	ion	ld 75-98-9 Date 06.11.2006
Remark 01.09.2006	: No additives present	
1.5 TOTAL QUANTITY		
1.6.1 LABELLING		
1.6.2 CLASSIFICATION		
1.6.3 PACKAGING		
1.7 USE PATTERN		
Type of use Category	: industrial : Chemical industry: used in synthesis	
Remark	: Primarily used as a chemical intermediate i	n the production of synthetic
01.09.2006	lubricants or hydraulic fluids.	
1.7.1 DETAILED USE PA	IUFACTURE	
1.8 REGULATORY MEA	ASURES	
1.8.1 OCCUPATIONAL E	XPOSURE LIMIT VALUES	
1.8.2 ACCEPTABLE RES	IDUES LEVELS	
1.8.3 WATER POLLUTIO	Ν	
1.8.4 MAJOR ACCIDENT	HAZARDS	
1.8.5 AIR POLLUTION		
1.8.6 LISTINGS E.G. CHE	EMICAL INVENTORIES	

1. General Information	ld 75-98-9 Date 06.11.200	6
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 Sublimation Method Year GLP Test substance	: = 35 °C : : other: calculated : 2003 : no	
Method Test condition	 Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04 Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Og 	jle.
	Joback's Method is described in Joback, K.G. 1982. A Unified Approach Physical Property Estimation Using Multivariate Statistical Techniques. The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J. Prausnitz and B.E. Poling, Eds.	to In .M.
Test substance Reliability Flag 01.09.2006	 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. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- (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 num listed under test substance. Critical study for SIDS endpoint 	ber (16)
2.2 BOILING POINT		
Value Decomposition Method Year GLP Test substance	: = 163 - 165 °C at 1013 hPa : : other: D1078/01 : 2003 : no data :	
Test substance Reliability Flag	 CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- (2) valid with restrictions Although the original data were not retrieved and reviewed for quality, th were developed following acceptable test methods and therefore considered reliable. Critical study for SIDS endpoint 	ey
01.09.2006		(9)
2.3 DENSITY		
Type Value Method Year GLP Test substance	 density = .91 g/cm³ at 20 °C other: ASTM D4052/86 equivalent 2003 no data 	

2. Physico-Chemi	cal Data	ld 75-98-9 Date 06.11.2006
Test substance Reliability	 CAS No. 75-98-9; Propanoic acid, 2,2-dimet (2) valid with restrictions Although the original data were not retrieved were developed following acceptable test me considered reliable. 	hyl- I and reviewed for quality, they ethods and therefore
Flag 01.09.2006	: Critical study for SIDS endpoint	(5
2.3.1 GRANULOMETR	Y	
2.4 VAPOUR PRESS	URE	
Value Decomposition Method Year GLP Test substance	 = 2.05 hPa at 25 °C other (calculated) 2003 	
Method	: Vapor pressure calculation by MPBPWIN ve method of Grain.	r. 1.40 using calculation
Remark Test substance Reliability	 EPIWIN is used and advocated by the US E estimation. CAS No. 75-98-9; Propanoic acid, 2,2-dimet (2) valid with restrictions The result is a calculated value based on the represents a potential vapor pressure for the purchase set interval water that a value based on the set interval water ba	PA for chemical property hyl- e chemical structure and e substance with the CAS
Flag 01.09.2006	: Critical study for SIDS endpoint	(14
	FEICIENT	
Partition coefficient Log pow pH value Method Year GLP Test substance	 octanol-water = 1.5 at 25 °C other (calculated) 2003 	
Pomark	 Value was provided by the experimental date CAS No. 75-98-9; Propanoic acid, 2,2-dimet 	abase of the EPIWIN program hyl-
Test substance Reliability	: (2) valid with restrictions Although the original data were not retrieved were developed following acceptable test me considered reliable.	and reviewed for quality, they ethods and therefore

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

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

2. Physico-Chemical Data

ld 75-98-9 Date 06.11.2006

concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
рКа	:	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)

(16)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value Type Method Year GLP Test substance	: = 62.8 °C : closed cup : other: TCC ASTM D56 : 2003 : no data :
Test substance Reliability	 CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- (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 15.09.2006	: Critical study for SIDS endpoint (9)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2. Physico-Chemical Data

ld 75-98-9 Date 06.11.2006

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant Method Year GLP Test substance	4.6 other: calculated 2003	
Method Remark	pKa calculation by SPARC 2003 using a Linux Calculation engine. 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 modele SPARC. This robust summary has a reliability rating of 2 because the are calculated and not measured.	d by e data
15.09.2006		(11)

2.13 VISCOSITY

Value Result Method Year GLP Test substance	= 3.6 - at 60 °C other: ASTM D445 2003 no data
Remark Test substance Reliability	 Value measured in cSt CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- (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

Туре	:	air			
Light source	÷	Sun light			
Relative intensity	-	based on intensity of	of sunlight		
INDIRECT PHOTOLYSIS	•		Si oannight		
Sensitizer	:	ОН			
Conc. of sensitizer	:	1500000 molecule/cm	3		
Rate constant	:	= .000000000010218	3 cm³/(molecule*sec)		
Degradation	:	% after			
Deg. product	÷	other (coloulated). Co	Jaulated values using AODWIN version 1.80		
Wethod	•	subroutine of the com	other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04		
Year	:	2003	pater program Er twirt version 0.04		
GLP	:				
Test substance	:				
Result	:	Atmospheric Oxidation	n Potential		
		In the environment, or degraded by several in transformation proces hydroxyl (OH-) radical organic compound rea atmospheric persisten	ganic chemicals emitted into the troposphere are mportant transformation processes. The dominant s for most compounds is the daylight reaction with s (Atkinson, 1988, 1989). The rate at which an acts with OH- radicals is a direct measure of its ce (Meylan and Howard, 1993).		
		AOPWIN estimates th reaction between phot chemicals. The rate c calculate atmospheric average atmospheric	e rate constant for the atmospheric, gas-phase tochemically produced hydroxyl radicals and organic constants estimated by the program are then used to half-lives for organic compounds based upon concentrations of hydroxyl radicals.		
		Since the reactions or atmospheric half-lives	ly take place in the presence of sunlight, the 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. Est for organic chemicals.	timation of gas-phase hydroxyl radical rate constants Environ. Toxicol. Chem. 7:435-442.		
		Atkinson, R. 1989. Kir the hydroxyl radical wi Monograph No. 1, Am	netics and mechanisms of the gas-phase reactions of ith organic compounds. J. Phys. Chem. Ref. Data er. Inst. Physics & Amer. Chem. Soc., NY.		
Test condition		Meylan, W.M. and P.H atmospheric gas-phas radicals and ozone. C Indirect photodegrada the structure-activity re	H. Howard. 1993. Computer estimation of the reaction rate of organic compounds with hydroxyl hemosphere 12:2293-2299. tion, or atmospheric oxidation potential, is based on elationship methods developed by R. Atkinson.		
		Temperature: 25°C			
		10 /	35		

ld 75-98-9

Date 06.11.2006

Test substance Reliability Flag 15.09.2006	 Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3 CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- (2) valid with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric h range for the test substance. Critical study for SIDS endpoint 	alf-life (15)
Type Light source Light spectrum Relative intensity Deg. product Method Year GLP Test substance	water nm based on intensity of sunlight other (calculated): Technical discussion	
Remark Result	 These data represent a key study for characterizing the potential of substances in the Neoacids C5 to C28 Category to undergo direct photodegradation. 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, The reaction process is initiated when light energy in a specific wave range elevates a molecule to an electronically excited state. Howeve excited state is competitive with various deactivation processes that 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 can result in the electronic excitation of an organic molecule. Light in range contains energy of the same order of magnitude as covalent b dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrare result only in vibrational and rotational transitions, which do not tend produce structural changes to a molecule.	1982). length r, the can nm, this ond ed) to
	The stratospheric ozone layer prevents UV light of less than 290 nm reaching the earth's surface. Therefore, only light at wavelengths bet 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 750 nm range is necessary, it is not always sufficient for a chemical transformation. Energy may be re-emitted from excited molecule by mechanisms other than chemical transformation resulting in no change to the parent molecule.	from ween e 290- o an ,
	A conservative approach to estimating a photochemical degradation to assume that degradation will occur in proportion to the amount of wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 19	rate is ight 977).
	Substances in the Neoacids C5 to C28 Category contain molecules t are oxygenated aliphatic compounds which will absorb UV light below nm (Boethling and Mackay, 2000) and will not undergo direct photoly Therefore, this fate process will not contribute to a measurable degra removal of chemical components in this category from the environme	hat v 220 vsis. adative ent.
	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 Chem	ical

3. Environmental	Fate and Pathways	ld 75-98-9 Date 06.11.2006
	Property Estimation Methods, McG USA.	raw-Hill Book Company, New York,
	Zepp, R. G. and D. M. Cline. 1977. Aqueous Environment, Environ. Sc	Rates of Direct Photolysis in the i. Technol., 11:359-366.
Test substance Flag 01.09.2006	 Boethling, R.S., Mackay, D. 2000. Methods for Chemicals, CRC Press Neoacids C5 to C28 Category mem Critical study for SIDS endpoint 	Handbook of Property Estimation s, Boca Raton, FL, USA. bers (4)
3.1.2 STABILITY IN W	ATER	
Type t1/2 pH4 t1/2 pH7 t1/2 pH9 Deg. product Method Year GLP Test substance	: abiotic : at °C : at °C : at °C : : other: technical discussion :	
Remark Result	 These data represent a key study for substances in the Neoacids C5 to C Hydrolysis as a Function of Molecu 	or characterising the potential of C28 Category to undergo hydrolysis. Iar Structure
	Hydrolysis of an organic molecule of with water (H2O) to form a new car bond is cleaved (Gould, 1959; Harr is referred to as a nucleophilic subs group being replaced by the incomi molecule.	occurs when a molecule (R-X) reacts bon-oxygen bond after the carbon-X is, 1982). Mechanistically, this reaction stitution reaction, where X is the leaving ng nucleophilic oxygen from the water
	Chemicals that are susecptible to h can be displaced by a nucleophilic have a potential to hydrolyze includ carboxylic acid esters and lactones sulfonic acid esters (Neely, 1985). renders a compound resistant to hy	ydrolysis contain functional groups that substitution reaction. Substances that le alkyl halides, amides, carbamates, , epoxides, phosphate esters, and The lack of a suitable leaving group rdrolysis.
	Aliphatic acids are resistant to hydr group that is hydrolytically reactive	olysis because they lack a functional (Harris, 1982).
	References:	
	Gould, E.S. (1959), Mechanism and Reinhart and Winston, New York, N	d Structure in Organic Chemistry, Holt, IY, USA.
	Harris, J.C. (1982), "Rate of Hydrol Reehl, and D.H. Rosenblatt, eds., H Estimation Methods, McGraw-Hill B	ysis," Chapter 7 in: W.J. Lyman, W.F. Handbook of Chemical Property Book Company, New York, NY, USA.
Test substance Conclusion	 Neely, W. B. 1985. Hydrolysis. In: V Environmental Exposure from Cher Boca Raton, FL, USA. Neoacids C5 to C28 Category mem Hydrolysis will not contribute to the environment. 	V. B. Neely and G. E. Blau, eds. nicals. Vol I., pp. 157-173. CRC Press, nbers removal of neoacids from the

3. Environmental Fa	te and Pathways	ld Date	75-98-9 06.11.2006	
Flag 01.09.2006	: Critical study for SIDS endpoint		(3)	
3.1.3 STABILITY IN SOIL				
3.2.1 MONITORING DATA				
3.2.2 FIELD STUDIES				
3.3.1 TRANSPORT BETW	EEN ENVIRONMENTAL COMPARTMENTS			
Type Media Air Water Soil Biota Soil Method YearMethod YearMethod 	 fugacity model level III other: air - sediment(s) - soil - water % (Fugacity Model Level I) % (Fugacity Model Level I)/III) % (Fugacity Model Level II/III) other: Calculation according Mackay, Level II 2003 The EQC Level III model is a steady state modetermining how the medium of release affect III fugacity allows non-equilibrium conditions is media as steady state, and illustrate important processes. Physicochemical input values for the model w EPIWIN Estimation v 3.04 program. Measure used where available and obtained from the I data from the equilibrium model provide basic partitioning behavior of chemicals between secompartments (i.e., air, water, soil, and sedim 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 - 72000 hrs This model was run assuming 100% discharges 	I odel that is ts environ to exist be at transpor vere calcu ed input va EPIWIN da c informati elected en hent).	s useful for mental fate. Level tween connected t and transformation lated using the alues were also atabase. Distribution on on the potential vironmental	
	Air - 0.78% Water - 98.7% Soil - 0.27% Sediment - 0.26%	·		
Test substance	: CAS No. 75-98-9; Propanoic acid, 2,2-dimeth 13 / 35	ıyl-		
ld 75-98-9 Date 06.11.2006

Reliability	: (2) valid with restrictions
	This robust summary has a reliability rating of 2 because the data are
	calculated and not measured.
Flag 18.00.2006	: Critical study for SIDS endpoint (12)
18.09.2008	(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
rear	: 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%
	Sealment - <0.01% Suspended Sed - <0.01%
	Biota - $<0.01\%$
Test substance Conclusion	 CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- 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.
Reliability	 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. (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 Inoculum Contact time Degradation Result Deg. product Method Year GLP Test substance	 aerobic activated sludge, domestic 28 day(s) = 24 (±) % after 28 day(s) inherently biodegradable OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test" 1996 yes
Remark Result	 Test Type: Manometric Respirometry Test 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.
Test condition	 % Degradation* Mean % Degradation Sample (day 28) (day 28) Test Material 18.9, 42.7, 10.7 24.1 Na Benzoate 98.9, 95.5 97.2 * replicate data 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.
Test substance Conclusion Reliability 18.09.2006	 All test vessels were stirred constantly for 28 days using magnetic stir bars and plates. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Test substance is considered not readily biodegradable. (1) valid without restriction (7)

3.6 BOD5, COD OR BOD5/COD RATIO

ld 75-98-9 Date 06.11.2006

3.7 BIOACCUMULATION

BCF Elimination Method Year GLP Test substance		= 3.16 other: calculated 2003
Method	:	Calculated values using BCFWIN version 2.13, a subroutine of the
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.
Toot substance		Log Kow used = 1.48
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 22.09.2006	:	Critical study for SIDS endpoint (5)

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type Species Exposure period Unit Limit test Analytical monitoring Method	 static Carassius auratus (Fish, fresh water) 96 hour(s) mg/l no yes other: Standard Methods for the Examination of Water and Wastewater Method #231, 1971
Year GLP Test substance	: 1979 : no :
Remark Result	 Statistical Method: Interpolation of graph of log of concentration (APHA 1971). LC50 = 380mg/L
Test condition	 Analytical method used was Total Organic Carbon or by extraction and subsequent GC analysis. 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.
Test substance Conclusion Reliability	 Fish Mean Wt.= 3.3 +/- 1.0g. Mean Total length = 6.2 +/-cm, Test Loading = 1.3 g of fish/L. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Test substance is considered to have low toxicity. (2) valid with restrictions Minimal data presented (i.e. lacking conc. series, analytical measurements, Dissolved Oxygen measurements).
riag	: Uritical study for SIDS endpoint

18.09.2006

(1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type Species Exposure period Unit Limit Test Analytical monitoring Method Year GLP Test substance	 static Daphnia magna (Crustacea) 48 hour(s) mg/l no other: USEPA -660/3-75-009 Methods for Acute Toxicity with Fish and Macroinvertebrates, and Amphibians, 1975 1977 no data
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

4. Ecotoxicity	ld 75-98-9 Date 06.11.2006
Test condition :	Test Concentration24 hr.48 hr.Positive Control00Negative Control0036 mg/L0060 mg/L00100 mg/L07170 mg/L713280 mg/L2093460 mg/L100100For 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
Test substance :	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 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 : 18.09.2006	Critical study for SIDS endpoint (2)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species Endpoint Exposure period Unit NOEC EC50 Limit test Analytical monitoring Method Year GLP Test substance		other algae: Pseudokirchneriella subcapitata biomass 72 hour(s) mg/l = 246 measured/nominal = 878 measured/nominal no yes OECD Guide-line 201 "Algae, Growth Inhibition Test" 2003 yes
Remark Result	:	Statistical Procedure - Proc regression procedure of SAS, Anova procedure of SAS for NOEC 72 hour EC50b=878 mg/L (biomass) 72 hour EC50gr=070 mg/L (growth rate)
		72 hour NOECb=246 mg/L (biomass) 72 hour NOECgr=246 mg/L (growth rate)
		Mean Cell Nominal Piamaga 72 hr
		Nominal Biomass - 72 hr Conc 72 hr
		18 / 35

4. Ecotoxicity			ld	75-98-9
-			Date	06.11.2006
	Conc. (mg/L) Control 62 125 250 500 1000	(% Inhibition) n/a 1.5 -3.0 -1.0 24 64	(cells/ml) 7.0 x105 6.9 x105 7.2 x105 7.1 x105 5.3 x105 2.4 x105	
Test conditionn/a - Not applicable note: a negative value indicates a stimulatory effect.Test condition: Individual test treatment solutions were prepared as Water Accom Fractions (WAFs). Test material was added to algal media in 2.0L aspirator bottles. The vessels were mixed on magnetic stir plates teflon coated stir bars for 23 hours at room temperature. After mix solutions were allowed to settle for one hour and the aqueous port WAF was removed from the bottom of the mixing vessel via the po- used for testing. Test vessels were 125ml glass Erlenmeyer flasks approximately 60 ml of treatment solution and inoculated with alga vessels were sealed with foam stoppers. Samples were taken dai counts. Four replicates were prepared for each treatment level. T algal concentration was 1.0 x 104 cells/ml. All test replicates were on a shaker table at 100 oscillations per minute during the study. was calculated as the area under the growth curve.		ater Accommodated redia in 2.0L c stir plates with e. After mixing the queous portion of the el via the port and meyer flasks with ed with algae. Test re taken daily for cell rent level. The initial licates were placed the study. Biomass		
	Nominal loading level Test treatments were Mean measured valu material was not dete	ls were 62, 125, 2 analyzed by GC es were 54.8, 12 ected in the contro	250, 500, and 10 FID on Day 0 ar 8, 246, 488 and 9 ol.	00 mg/L nd at termination. 979 mg/L. The test
Test substance	Test temperature was 7586 Lux. The pH wa 7.5 at test termination CAS No. 75-98-9; Pro	s 23.4 Deg. C. L as 7.4 to 7.6 at te n. opanoic acid, 2,2	ighting was conti est initiation and r -dimethyl-	nuous at 7229 to ranged from 7.1 to
Reliability Flag	: (1) valid without restri : Critical study for SIDS	iction S endpoint		
18.09.2006				(8)
4.4 TOXICITY TO MI	CROORGANISMS E.G. BAC	TERIA		
4.5.1 CHRONIC TOXIC	ITY TO FISH			
4.5.2 CHRONIC TOXIC	ITY TO AQUATIC INVERTE	BRATES		
4.6.1 TOXICITY TO SE	DIMENT DWELLING ORGA	NISMS		

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4. Ecotoxicity Id 75-98-9 Date 06.11.2006			
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. Toxicity

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type Value Species Strain Sex Number of animals Vehicle Doses Method Year GLP Test substance		LD50 = 2000 mg/kg bw rat Sprague-Dawley male 5 other: none other 1964 no
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. LD50= 2000 mg/kg (CL: 830 to 4820 mg/kg)
Test condition	:	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 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
Dell'al l'Iter		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)

(6)

5.1.2 ACUTE INHALATION TOXICITY

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

ld 75-98-9 Date 06.11.2006

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.		
esult	: Rat > 4.0 mg/L		
est 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.		
est substance conclusion	 CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- has a moderate order of inhalation toxicity in 		
Doliobility	rogents.		
Reliability	No vapor concentration verification (analytical). Study was performed pre-		
	GLF Tegulations.		
-lag	: Childai study for SIDS endpoint		
8.09.2006	(6)		
Гуре	: LC50		
/alue	: < 4 mg/l		
pecies	: mouse		
Strain	: other: Swiss albino		
Sex	: male		
Number of animals	: 10		
/ehicle	:		
Doses	:		
Exposure time	: 6 hour(s)		
lethod	: other		
(ear	: 1964		
GLP	: no		
Test substance	:		
lemark	: 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		

5. Toxicity

5. Toxicity	Id 75-98-9
-	Date 06.11.2006
	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.
Booulé	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.
Test condition	 Mouse LCSU < 4.0 mg/L 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 Value Species Strain Sex Number of animals Vehicle Doses Method Year GLP Test substance	 LD50 = 3160 mg/kg bw rabbit other: Albino male/female 4 other: none 50, 200, 794, 3160 mg/kg (single dose) other 1964 no
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.

5. Toxicity	ld 75-98-9
2	Date 06.11.2006
	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	$\pm LD50 = 3160 \text{ mg/kg}$
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 Concentration Exposure Exposure time Number of animals Vehicle PDII Result Classification Method Year GLP Test substance		rabbit Semiocclusive 24 hour(s) 4 other: none
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

5. Toxicity	Id 75-98-9
	Date 06.11.2006
	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 Reliability	: CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Rendomey	Study performed Pre-GLP.
Flag 18.09.2006	: Critical study for SIDS endpoint
10.03.2000	(0)

5.2.2 EYE IRRITATION

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

, ,	Date 06.11.2006
	eves were examined and scored for ocular reactions according to the
	Draize Standard Eve Irritation Grading Scale.
Test substance	· CAS No. 75-98-9: Propanoic acid. 2.2-dimethyl-
Poliobility	(2) volid with restrictions
Reliability	. (2) valid with restrictions
	Study performed pre-GLP.
Flag	: Critical study for SIDS enapoint
16.10.2006	(
5.3 SENSITIZATION	
Туре	: Guinea pig maximization test
Species	: auinea pia
Number of animals	
Vehicle	
Docult	· not sensitizing
	. not sensulling
Classification	: All a Mars and D Kings A.M. Lib at Deviatel, 50, 4000
wethoa	: other: Magnusson, B. Kilgman, 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
Reliability	Although the original date was not retrieved and reviewed for quality they
	Although the original data was not retrieved and reviewed for quality, they were developed following accordable test methods and therefore
	were developed following acceptable lest methods and therefore
	considered reliable.
Flag	: Critical study for SIDS endpoint
Flag 21.09.2006	: Critical study for SIDS endpoint (1
Flag 21.09.2006	: Critical study for SIDS endpoint (1
Flag 21.09.2006 5.4 REPEATED DOSE	: Critical study for SIDS endpoint (1
Flag 21.09.2006 5.4 REPEATED DOSE	: Critical study for SIDS endpoint (1 TOXICITY
Flag 21.09.2006 5.4 REPEATED DOSE	: Critical study for SIDS endpoint (1 TOXICITY : rabbit
Flag 21.09.2006 5.4 REPEATED DOSE Type Species Sex	: Critical study for SIDS endpoint (1 TOXICITY : rabbit : male
Flag 21.09.2006 5.4 REPEATED DOSE Type Species Sex Strain	: Critical study for SIDS endpoint (1 TOXICITY : rabbit : male : other: Albino
Flag 21.09.2006 5.4 REPEATED DOSE Type Species Sex Strain Route of admin	: Critical study for SIDS endpoint (1 TOXICITY : rabbit : male : other: Albino : dermal
Flag 21.09.2006 5.4 REPEATED DOSE Type Species Sex Strain Route of admin. Exposure period	: Critical study for SIDS endpoint (1 TOXICITY : rabbit : male : other: Albino : dermal
Flag 21.09.2006 5.4 REPEATED DOSE 5.4 Species Sex Strain Route of admin. Exposure period Frequency of treatm	: Critical study for SIDS endpoint (1 TOXICITY : rabbit : male : other: Albino : dermal : 10 applications with a two-day rest between the 5th and 6th applications
Flag 21.09.2006 5.4 REPEATED DOSE 5.4 Species Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period	: Critical study for SIDS endpoint (1 TOXICITY : rabbit : male : other: Albino : dermal : 10 applications with a two-day rest between the 5th and 6th applications
Flag 21.09.2006 5.4 REPEATED DOSE 5.4 Species Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period	 Critical study for SIDS endpoint (1 TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications
Flag 21.09.2006 5.4 REPEATED DOSE 5.4 REPEATED DOSE 5.4 Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses	 Critical study for SIDS endpoint (1 TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other learnered Alebel (IDA) was a devisite the 2 schedule and the solution in the 3 schedule and 3 schedule and the 3 schedule and 3 schedule and the 3 schedule and 3 schedu
Flag 21.09.2006 5.4 REPEATED DOSE 5.4 REPEATED DOSE 5.4 Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group	 Critical study for SIDS endpoint (1 TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of
Flag 21.09.2006 5.4 REPEATED DOSE Type Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group	 Critical study for SIDS endpoint (1 TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application.
Flag 21.09.2006 5.4 REPEATED DOSE 5.4 REPEATED DOSE 5.4 Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL	 Critical study for SIDS endpoint (1) TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg
Flag 21.09.2006 5.4 REPEATED DOSE 5.4 REPEATED DOSE 5.4 Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method	 Critical study for SIDS endpoint (1) TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other
Flag 21.09.2006 5.4 REPEATED DOSE 5.4 REPEATED DOSE 5.4 Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method Year	 Critical study for SIDS endpoint (1) TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other 1964
Flag 21.09.2006 5.4 REPEATED DOSE 5.4 REPEATED DOSE 5.4 Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method Year GLP	 Critical study for SIDS endpoint (1) TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other 1964 no
Flag 21.09.2006 5.4 REPEATED DOSE Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method Year GLP Test substance	 Critical study for SIDS endpoint (1) TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other 1964 no
Flag 21.09.2006 5.4 REPEATED DOSE Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method Year GLP Test substance Remark	 Critical study for SIDS endpoint (1 TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other 1964 no No. of animals/sex/dose: 4
Flag 21.09.2006 5.4 REPEATED DOSE Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method Year GLP Test substance Remark	 Critical study for SIDS endpoint (1) TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other 1964 no No. of animals/sex/dose: 4 Route of administration: Dermal
Flag 21.09.2006 5.4 REPEATED DOSE Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method Year GLP Test substance Remark	 Critical study for SIDS endpoint (1 TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other 1964 no No. of animals/sex/dose: 4 Route of administration: Dermal Vehicle: Isopropyl Alcohol (IPA)
Flag 21.09.2006 5.4 REPEATED DOSE Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method Year GLP Test substance Remark	 Critical study for SIDS endpoint (1) TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other 1964 no No. of animals/sex/dose: 4 Route of administration: Dermal Vehicle: Isopropyl Alcohol (IPA) Statistical method: Not reported
Flag 21.09.2006 5.4 REPEATED DOSE Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method Year GLP Test substance Remark	 Critical study for SIDS endpoint (1 TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other 1964 no Ino
Flag 21.09.2006 5.4 REPEATED DOSE Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method Year GLP Test substance Remark	 Critical study for SIDS endpoint (1 TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other 1964 no Ino Ino<
Flag 21.09.2006 5.4 REPEATED DOSE Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method Year GLP Test substance Remark	 Critical study for SIDS endpoint (1 TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other 1964 no Ino Statistical method: Not reported The control animals exhibited normal appearance and behavior throughou the study with the exception of nasal discharge in one animal and diarrhead in another.
Flag 21.09.2006 5.4 REPEATED DOSE Species Sex Strain Route of admin. Exposure period Frequency of treatm. Post exposure period Doses Control group NOAEL Method Year GLP Test substance Remark	 Critical study for SIDS endpoint (1) TOXICITY rabbit male other: Albino dermal 10 applications with a two-day rest between the 5th and 6th applications 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol other: Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. = 300 mg/kg other 1964 no Ino Ino 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 diarrheat in another. Slight body weight loss was observed during the first week, but the exception of nasal discharge in one animal and diarrheat in another. Slight body weight loss was observed during the first week, but the exception of nasal discharge in one animal and diarrheat in another. Slight body weight loss was observed during the first week, but the exception of nasal discharge in one animal and diarrheat in another.

Γ

5. Toxicity	ld 75-98-9
	Date 06.11.2006
	at gross necropsy. Repeat applications did not cause any histopathological alterations to the liver or kidney of the rabbits.
Result	 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. For systemic effects: NOAEL = 300 mg/kg
Test condition	 Propanoic acid, 2,2-dimethyl- produced moderate to severe skin irritation. 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 Conclusion	 CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- 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 Critical study for SIDS endpoint
18.09.2006	(10)
Туре	:
Species	: rat • male/female
Strain	: Fischer 344
Route of admin.	: gavage
Exposure period	:
Frequency of treatm.	: 28 consecutive days
Post exposure period	\therefore 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 Test substance	: yes
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.

5. Toxicity	ld 75-98-9
-	Date 06.11.2006
	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
	these changes correlated with histopathology effects and were due to local irritation and increase in functional demand.
	Number of animals: 7/sex/dose
Test substance	Vehicle: Water/polyethylene glycol 200 50/50 (v/v) CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl-
Conclusion	: Propanoic acid, 2,2-dimethyl- has a low order of sub-chronic toxicity.
Poliobility	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.
Flag	: Critical study for SIDS endpoint
18.09.2006	(20)
5.5 GENETIC TOXICIT	Y 'IN VITRO'
Туре	: 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	
Desult	
Result	: negative
Result Method Yoar	negative
Result Method Year GI P	 negative 1978 no
Result Method Year GLP Test substance	negative 1978 no
Result Method Year GLP Test substance Remark	 with and without negative 1978 no Plate incorporation assay
Result Method Year GLP Test substance Remark	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction
Result Method Year GLP Test substance Remark	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified)
Result Method Year GLP Test substance Remark Result	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9
Result Method Year GLP Test substance Remark Result Test substance	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9: Propanoic acid. 2 2-dimethyl-
Result Method Year GLP Test substance Remark Result Test substance Conclusion	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S.
Result Method Year GLP Test substance Remark Result Test substance Conclusion	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay.
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (2) valid with restrictions
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (2) valid with restrictions Although the original data was not retrieved and reviewed for quality, they
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (2) valid with restrictions Although the original data was not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (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. Critical ctudy for SIDS andpoint
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability Flag 21.09.2006	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (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. Critical study for SIDS endpoint
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability Flag 21.09.2006 Type	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (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. Critical study for SIDS endpoint (19)
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability Flag 21.09.2006 Type System of testing	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (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. Critical study for SIDS endpoint (19) Yeast gene mutation assay other: Yeast with and without metabolic activation
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability Flag 21.09.2006 Type System of testing Test concentration	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (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. Critical study for SIDS endpoint (19) Yeast gene mutation assay other: Yeast with and without metabolic activation 0.01, 0.1, 0.5, 1.0, 5.0 mg/ml ± S9. All diluted in DMSO
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability Flag 21.09.2006 Type System of testing Test concentration Cycotoxic concentr.	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (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. Critical study for SIDS endpoint (19) Yeast gene mutation assay other: Yeast with and without metabolic activation 0.01, 0.1, 0.5, 1.0, 5.0 mg/ml ± S9. All diluted in DMSO
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability Flag 21.09.2006 Type System of testing Test concentration Cycotoxic concentr.	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (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. Critical study for SIDS endpoint (19) Yeast gene mutation assay other: Yeast with and without metabolic activation 0.01, 0.1, 0.5, 1.0, 5.0 mg/ml ± S9. All diluted in DMSO
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability Flag 21.09.2006 Type System of testing Test concentration Cycotoxic concentr. Metabolic activation Result	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (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. Critical study for SIDS endpoint (19) Yeast gene mutation assay other: Yeast with and without metabolic activation 0.01, 0.1, 0.5, 1.0, 5.0 mg/ml ± S9. All diluted in DMSO with and without negative
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability Flag 21.09.2006 Type System of testing Test concentration Cycotoxic concentr. Metabolic activation Result Method	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (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. Critical study for SIDS endpoint Yeast gene mutation assay other: Yeast with and without metabolic activation 0.01, 0.1, 0.5, 1.0, 5.0 mg/ml ± S9. All diluted in DMSO with and without negative
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability Flag 21.09.2006 Type System of testing Test concentration Cycotoxic concentr. Metabolic activation Result Method Year GLP	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (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. Critical study for SIDS endpoint (19) Yeast gene mutation assay other: Yeast with and without metabolic activation 0.01, 0.1, 0.5, 1.0, 5.0 mg/ml ± S9. All diluted in DMSO with and without negative 1978 po
Result Method Year GLP Test substance Remark Result Test substance Conclusion Reliability Flag 21.09.2006 Type System of testing Test concentration Cycotoxic concentr. Metabolic activation Result Method Year GLP	 with and without negative 1978 no Plate incorporation assay Species/strain: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified) There was no increase in reverse mutation rate in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in strains of the bacteria S. typhimurium or E. coli under conditions of this assay. (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. Critical study for SIDS endpoint Yeast gene mutation assay other: Yeast with and without metabolic activation 0.01, 0.1, 0.5, 1.0, 5.0 mg/ml ± S9. All diluted in DMSO with and without negative 1978 no

5. Toxicity	ld 75-98-9 Date 06.11.2006	
Remark	Liquid suspension assay Species/strain: Saccharomyces cerevisiae JD1 Species/cell type: Rat liver (S9) fraction Induced: Aroclor 1254 induced (treatment not specified)	
Result Test substance Conclusion Reliability	Statistical methods were not reported There was no increase in the mitotic gene conversion frequency in either the presence or absence of S9. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not mutagenic in Saccharomyces cerevisiae JD1 under conditions of this assay. (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	considered reliable. (19)	
Type System of testing Test concentration Cycotoxic concentr. Metabolic activation Result Method Year GLP Test substance	Chromosomal aberration test Cultured rat liver cell line 0, 125, 250, 500 μ g/ml ± S9. All diluted in DMSO with and without negative 1978 no	
Remark	Rat liver cells (RL1) with and without metabolic activation.	
	At 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.	
Test substance Conclusion Reliability	 treated cells. CAS No. 75-98-9; Propanoic acid, 2,2-dimethyl- Propanoic acid, 2,2-dimethyl- is not genotoxic in rat liver cells in vitro under conditions of this assay. (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 21.09.2006	Critical study for SIDS endpoint (19)	

5.6 GENETIC TOXICITY 'IN VIVO'

5. Toxicity

ld 75-98-9 Date 06.11.2006

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. Analyt. Meth. for Detection and Identification	

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. E f	f. Against Target Org. and Intended Uses	ld Date	75-98-9 06.11.2006
7.1	FUNCTION		
7.2	EFFECTS ON ORGANISMS TO BE CONTROLLED		
7.3	ORGANISMS TO BE PROTECTED		
7.4	USER		
7.5	RESISTANCE		

8.	Meas.	Nec.	to Prot.	Man,	Animals,	Environment
----	-------	------	----------	------	----------	-------------

- 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

9. References

- (1) Bridie, A.L. et al. 1979. The Acute Toxicity Test of some Petrochemicals to Goldfish. Water Research Vol. 13.
- (2) EG&G Bionomics, Wareham, Mass.
- (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) Exxon Biomedical Sciences Inc. Ready Biodegradability: OECD 301F Manometric Respirometry Test. 136894A.
- (8) ExxonMobil Biomedical Sciences, Inc. (EMBSI, 2003). Alga, Growth Inhibition Test. Study No. 145467. Unpublished report.
- (9) ExxonMobil Chemical Company (2003). Neo Pentanoic Acid. Unpublished internal data.
- (10) Hazleton Laboratories, Inc. (1964) "Repeated Dermal Application Rabbits," Unpublished report.
- (11) 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.
- (12) Mackay D, DiGuardo A, Paterson S and Cowan C (1997). EQC Model ver. 1.01, available from the Environmental Centre, Trent University, Canada.
- (13) Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model ver. 2.02, available from the Environmental Centre, Trent University, Canada.
- (14) Meylan M (1994-1999). Calculation program contained in EPIWIN (Estimate ver. 3.04) available from SRC. Syracuse Research Corporation, Syracuse, New York, USA.
- Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN.
 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
- Meylan, M., SRC 1994-1999. WSKOWWIN is contained in the computer program EPIWIN.
 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
- Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN.
 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
- (18) Shell Research Ltd. (1977). Toxicology of Fine Chemicals: Acute Toxicity, Skin and Eye Irritancy and Skin Sensitizing Potential of Pivalic Acid. Unpublished report.
- (19) Shell Research Ltd. (1978) Toxicity studies with pivalic acid: in vitro mutation studies. (Tunstall Toxicology Laboratory) Unpublished report.
- (20) Shell Research Ltd.(1990) Pivalic acid: A 28 day oral toxicity study in rats. Shell Research Ltd, Sittingbourne, England. Unpublished report.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-16393D	
	-



2006 NOV 14 AM 10: 55

IUCLID

Data Set

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

1. General Information

ld 95823-36-2 Date 06.11.2006

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

erre	эе	text
2	ee tre	e tree

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 Molecular weight Petrol class	::	C7H14O2 130.19
Flag 26.09.2006	:	Critical study for SIDS endpoint

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid

T. General informa	tion Date 06.11.2006
Purity Colour Odour	: : :
Remark	 CAS Registry Number, Name, and General Structure for Members of the Neoacids C5 to C28 Category and Analogue Substances:
26.09.2006	CAS RN: 95823-36-2 TSCA Name: Carboxylic acids, C6-8-neo- R length (C number): C7 Structure of R: Linear Category Member: Yes
1.1.2 SPECTRA	
1.2 SYNONYMS AND	TRADENAMES
2-ethyl-2-methylbutanc	ic acid
26.09.2006	
neoheptanoic acid	
26.00.2006	
20.09.2000	
1.3 IMPURITIES	
Purity CAS-No	 typical for marketed substance 95823-36-2
EC-No	:
EINECS-Name Molecular formula	: : C7H14O2
Value	: = 97 % w/w
26.09.2006	
Purity type CAS-No EC-No FINECS-Name	 typical for marketed substance 95823-36-2 .
Molecular formula Value Function of additive	C7H14O2
	. No odditivoo procent

1. General Information	ld Date	95823-36-2 06.11.2006
1.6.1 LABELLING		
1.6.2 CLASSIFICATION		
1.6.3 PACKAGING		
1.7 USE PATTERN		
Type of use: industrialCategory: Chemical industry: used in synthesis		
Remark: Primarily used as a component of synthetic lul26.09.2006	bricants o	or hydraulic fluids.
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. Ge	neral Information	ld Date	95823-36-2 06.11.2006
1.10	SOURCE OF EXPOSURE		
1.11	ADDITIONAL REMARKS		
1.12	LAST LITERATURE SEARCH		
1.13	REVIEWS		

2.1 MELTING POINT

Value Sublimation Method Year GLP Test substance	: = 24.6 °C : : other: ASTM D97 : 2003 : no data
Test substance Reliability	 CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (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 26.09.2006	: Critical study for SIDS endpoint (14)
2.2 BOILING POINT	
Value Decomposition Method Year GLP Test substance	: = 207 - 210 °C at : : other: D1078/01 : 2003 : no data
Test substance Reliability Flag 26.09.2006	 CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (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. Critical study for SIDS endpoint (14)
2.3 DENSITY	
Type Value Method Year GLP Test substance	<pre>density = .93 g/cm³ at 20 °C 2003 no data</pre>
Test substance Reliability	 CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (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. Critical study for SLDS and point
27.09.2006	. Childai study for SIDS enupoint (14)
2.3.1 GRANULOMETRY	

2. Physico-Chemical Data

(5)

2.4 VAPOUR PRESSURE

Value Decomposition Method Year GLP Test substance	 = .325 hPa at 25 °C other (calculated) 2003
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 27.09.2006	: Critical study for SIDS endpoint

2.5 PARTITION COEFFICIENT

Partition coefficient Log pow pH value Method Year GLP Test substance	 octanol-water = 2.4 at 25 °C other (calculated) 2003
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.	:
рКа	: 4.7 at 25 °C
Description	:
Stable	:
Deg. product	:

2. Physico-Chemical Data

Method Year GLP Test substance	 other: calculated 2003 : 	
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)
27.09.2006		

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value Type Method Year GLP Test substance	 = 97 °C closed cup other: TCC ASTM D56 2003 no data
Test substance Reliability Flag 27.09.2006	 CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (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. Critical study for SIDS endpoint

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2. Physico-Chemical Data

(14)

2.12 DISSOCIATION CONSTANT

Acid-base constant Method Year GLP Test substance	: : :	4.7 other: calculated 2003
Method Remark	:	pKa calculation by SPARC 2003 using a Linux calculation engine. SPARC On-line calculator can be accessed at
Test substance Reliability 27.09.2006	:	http://ibmlc2.chem.uga.edu/sparc/index.cfm CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (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)
2.13 VISCOSITY		
Value Result Method Year GLP Test substance		= 9 - at 20 °C other: ASTM D445 2003
Remark Test substance Reliability	:	Value measured in cSt CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (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

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type Light source Light spectrum Relative intensity INDIRECT PHOTOLYSIS Sensitizer Conc. of sensitizer Rate constant Degradation Deg. product Method Year GLP Test substance		Sun light nm based on intensity of OH 1500000 molecule/cm = .000000000033 cm % after other (calculated): Ca subroutine of the comp 2003	of sunlight ³ n³/(molecule*sec) Ilculated values using AOPWIN version 1.89, a puter program EPIWIN version 3.04
Result	:	Atmospheric Oxidation	n Potential
		In the environment, or degraded by several in transformation process hydroxyl (OH-) radical organic compound rea atmospheric persisten	ganic chemicals emitted into the troposphere are mportant transformation processes. The dominant s for most compounds is the daylight reaction with s (Atkinson, 1988, 1989). The rate at which an acts with OH- radicals is a direct measure of its ce (Meylan and Howard, 1993).
		AOPWIN estimates th reaction between phot chemicals. The rate c calculate atmospheric average atmospheric of	e rate constant for the atmospheric, gas-phase tochemically produced hydroxyl radicals and organic constants estimated by the program are then used to half-lives for organic compounds based upon concentrations of hydroxyl radicals.
		Since the reactions on atmospheric half-lives	nly take place in the presence of sunlight, the are normalized for a 12-hour day.
		Calculated* half-life (days)	OH- Rate Constant (cm3/molecule-sec)
		3.2	3.2965 E-12
		References:	
		timation of gas-phase hydroxyl radical rate constants 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.	
Test condition	:	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. Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.	
Temperature: 25°C			
		10 / 3	36

ld 95823-36-2

Date 06.11.2006

Test substance Reliability	 Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3 CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (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 27.09.2006	: Critical study for SIDS endpoint (5)
Type Light source Light spectrum Relative intensity Deg. product Method Year GLP Test substance	water nm based on intensity of sunlight other (calculated): Technical discussion
Remark	 These data represent a key study for characterizing the potential of substances in the Neoacids C5 to C28 Category to undergo direct
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 11 / 36

3. Environmenta	I Fate and Pathways	ld 95823-36-2
	· · · · · · · · · · · · · · · · · · ·	Date 06.11.2006
	Property Estimation Methods, McGra USA.	w-Hill Book Company, New York,
	Zepp, R. G. and D. M. Cline. 1977. R Aqueous Environment, Environ. Sci.	ates of Direct Photolysis in the Technol., 11:359-366.
Tost substance	Boethling, R.S., Mackay, D. 2000. Ha Methods for Chemicals, CRC Press,	andbook of Property Estimation Boca Raton, FL, USA.
Flag 01.09.2006	: Critical study for SIDS endpoint	(4)
3.1.2 STABILITY IN W	IATER	
Туре		
t1/2 pH4	: at °C	
t1/2 pH7	: at °C	
t1/2 pH9	: at °C	
Deg. product	: other: technical discussion	
Year		
GLP	:	
Test substance	:	
Remark	: These data represent a key study for substances in the Neoacids C5 to C2	characterising the potential of 8 Category to undergo hydrolysis.
Result	: Hydrolysis as a Function of Molecular	r Structure
	Hydrolysis of an organic molecule occ with water (H2O) to form a new carbo bond is cleaved (Gould, 1959; Harris, is referred to as a nucleophilic substit group being replaced by the incoming molecule.	curs when a molecule (R-X) reacts on-oxygen bond after the carbon-X 1982). Mechanistically, this reaction ution reaction, where X is the leaving nucleophilic oxygen from the water
	Chemicals that are susecptible to hydronycologic can be displaced by a nucleophilic surplice a potential to hydrolyze include carboxylic acid esters and lactones, esulfonic acid esters (Neely, 1985). The renders a compound resistant to hydronycologic carboxylice carboxylice carboxylice carboxylice carboxylice acid esters (Neely, 1985).	trolysis contain functional groups that bstitution reaction. Substances that alkyl halides, amides, carbamates, epoxides, phosphate esters, and e lack of a suitable leaving group rolysis.
	Aliphatic acids are resistant to hydroly group that is hydrolytically reactive (H	ysis because they lack a functional larris, 1982).
	References:	
	Gould, E.S. (1959), Mechanism and S Reinhart and Winston, New York, NY	Structure in Organic Chemistry, Holt, , USA.
	Harris, J.C. (1982), "Rate of Hydrolys Reehl, and D.H. Rosenblatt, eds., Ha Estimation Methods, McGraw-Hill Boo	is," Chapter 7 in: W.J. Lyman, W.F. ndbook of Chemical Property ok Company, New York, NY, USA.
Test substance	Neely, W. B. 1985. Hydrolysis. In: W. Environmental Exposure from Chemic Boca Raton, FL, USA.	B. Neely and G. E. Blau, eds. cals. Vol I., pp. 157-173. CRC Press,
Conclusion	 Hydrolysis will not contribute to the re environment. 	ens emoval of neoacids from the

3. Environmental Fate	e and Pathways	ld ate	95823-36-2 06.11.2006	
Flag : 01.09.2006	Critical study for SIDS endpoint			(3)
3.1.3 STABILITY IN SOIL				
3.2.1 MONITORING DATA				
3.2.2 FIELD STUDIES				
3.3.1 TRANSPORT BETWEE	EN ENVIRONMENTAL COMPARTMENTS			
Type:Media:Air:Water:Soil:Biota:Soil:Method:Year:Method:Soil:Method:Soil:Method:Method:Soil:Method:Soil:Soil:Method:Soil:Soil:Method:Soil: <trt< td=""><td>fugacity model level III other: air - sediment(s) - soil - water % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) other: Calculation according Mackay, Level III 2003 The EQC Level III model is a steady state model that determining how the medium of release affects envi III fugacity allows non-equilibrium conditions to exis media as steady state, and illustrate important trans- processes. Physicochemical input values for the model were ca EPIWIN Estimation v 3.04 program. Measured inpu- used where available and obtained from the EPIWII data from the equilibrium model provide basic inforr partitioning behavior of chemicals between selected 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 Soil - 7200 hrs Sediment - 72000 hrs This model was run assuming 100% discharge to w</td><td>at is ironi t be spor alcul ut va matiu d en vater</td><th>useful for mental fate. Leve tween connected t and transformati ated using the lues were also atabase. Distributi on on the potentia vironmental</th><td>श on al</td></trt<>	fugacity model level III other: air - sediment(s) - soil - water % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) other: Calculation according Mackay, Level III 2003 The EQC Level III model is a steady state model that determining how the medium of release affects envi III fugacity allows non-equilibrium conditions to exis media as steady state, and illustrate important trans- processes. Physicochemical input values for the model were ca EPIWIN Estimation v 3.04 program. Measured inpu- used where available and obtained from the EPIWII data from the equilibrium model provide basic inforr partitioning behavior of chemicals between selected 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 Soil - 7200 hrs Sediment - 72000 hrs This model was run assuming 100% discharge to w	at is ironi t be spor alcul ut va matiu d en vater	useful for mental fate. Leve tween connected t and transformati ated using the lues were also atabase. Distributi on on the potentia vironmental	श on al
	Air - 0.71% Water - 98.2% Soil - 0.39% Sediment - 0.74%			
Test substance :	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo 13 / 36			

Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured. Critical study for SIDS endpoint
27.09.2006	•	(17)
Type Media Air Water Soil Biota Soil Method Year		fugacity model level I other: air - biota - sediment(s) - soil - water % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) other: Calculation according Mackay, Level I 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).
Desett		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 Conclusion	:	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo 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.
Poliability		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.
nenaviiity	•	This robust summary has a reliability rating of 2 because the data are
Flag	:	calculated and not measured. 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 Inoculum Contact time Degradation Result Deg. product Method Year GLP Test substance	 aerobic activated sludge, domestic 28 day(s) = 44 (±) % after 28 day(s) inherently biodegradable OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test" 1996 yes
Remark Result	 Test Type: Manometric Respirometry Test 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. % Degradation* Mean % Degradation
	Sample (day 28) (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 Elimination Method Year GLP Test substance	: = 3.16 : : other: calculated : 2003
Method	: Calculated values using BCFWIN version 2.13, a subroutine of the
Test condition	 Computer program EPIWIN Version 3.04 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.
Test substance Reliability	 Log Kow used = 2.43 CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (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 27.09.2006	: Critical study for SIDS endpoint (5)

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type Species Exposure period Unit LC50 Limit test Analytical monitoring Method Year GLP Test substance	 flow through Pimephales promelas (Fish, fresh water) 96 hour(s) mg/l = 630 measured/nominal no yes EPA OTS 797.1400 1993 yes
Remark Result	 Statistical Method: Graphical (EPA-600/4-90-027) LC50 = 630mg/L, based upon measured concentrations.
Test condition	 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 12.5 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 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.
Test substance Conclusion Reliability Flag 27.09.2006	 Fish Mean Wt.= 0.065g. Mean Total length = 1.6cm, Test Loading = 0.11 g of fish/L. CAS No. 95823-36-2; Carboxylic acids, C6-8-neo Test substance is considered low toxicity. (1) valid without restriction Critical study for SIDS endpoint (11)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Туре	:	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		

4. Ecotoxicity	ld 95823-36-2 Date 06.11.2006	
Year GLP Test substance	: 1993 : yes :	
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	
Test condition	 Statistical Method = Probit (Finney) of SAS 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 substance	 Test organisms were <24 hrs at initiation from 15 day old adults. CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (read across from Heptanoic C7 acid - approximately 70% n-heptanoic acid, 30% iso- 	
Conclusion Reliability Flag 27.09.2006	neptanoic acid). : Test substance is considered low toxicity : (1) valid without restriction : Critical study for SIDS endpoint (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	:	-

4. Ecotoxicity	ld 95823-36-2 Date 06.11.2006
Remark : Result :	Statistical Method: Linear Interpolation 96 hour EC50 = $6.49mg/L$ (95% Cl 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 lonization Detection (GC-FID).Nominal Conc. Measured Conc. Mean Cells % Inhibition (mg/L) Day 0 (mg/L) at 96 hr at 96 hr Control 0 2.3 E6 - 3.12 3.03 $2.3 E6$ 0
Test substance:Conclusion:Reliability:Flag:19.10.2006	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. CAS No. 95823-36-2; Carboxylic acids, C6-8-neo Test substance is considered moderately toxic. (1) valid without restriction Critical study for SIDS endpoint (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	:			

4. Ecotoxicity	ld 95823-36-2 Date 06.11.2006	
Test substance	:	
Result		
Rooun	The No Observed Effect Concentration (NOEC) and Lowest Observed Effect Concentration (LOEC) for Adult Immobilization was 4.78 and 10. mg/L, respectively. The NOEC and LOEC values for Offspring per Adu were 4.78 and 10.1 mg/L, respectively.	.1 Jlt
	The Maximum Acceptable Toxicant Concentration (MATC), which is th maximum concentration at which the test chemical can be present and be toxic to the organism, was 6.93 mg/L, and was based on adult immobilization and number of young per adult.	e not
Test condition	 Statistical Methods = Probit (Finney) of SAS; and Duncan's Multiple Ra Test of SAS. The study was conducted under flow-through conditions for a period of days. A stock solution was prepared daily at a nominal concentration of mg/L. The stock solution was delivered to the test chambers via a dilu- 	ange 21 of 5(ter
	system where it prepared test treatments at nominal levels of 0, 3.12, 6 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 wa 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 cov Test organisms were fed green algae and a yeast/salmon starter/cereat leaves mixture daily.	3.25 3, IS Versi al
	Forty daphnids (10 per 4 replicates) were tested at each concentration level.	
	Solubility of C7 acid = 3200mg/l.	
	Diluent Alkalinity = 35 mg CaCO3/I Hardness = 100 mg CaCO3/I Conductance = 236 umhos	
Test substance	 TOC = 1.1 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 SI	EDIMENT DWELLING ORGANISMS	
4.6.2 TOXICITY TO TE	RRESTRIAL PLANTS	

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4. Ecotoxicity

ld 95823-36-2 Date 06.11.2006

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5. Toxicity

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type Value Species Strain Sex Number of animals Vehicle Doses Method Year GLP Test substance		LD50 = 1860 mg/kg bw rat Sprague-Dawley male 5 other: none other 1964 no	
Remark	:	Route of administration: Gastric Intubation Frequency of Treatment: Single Dose Dose/Concentration Levels: 34.6, 120, 417, 1450, 5000, and 10000 mg, 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	/kg
Result	:	LD50= 1860 ma/ka	
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	<u> </u>
27.09.2006			(7)

5.1.2 ACUTE INHALATION TOXICITY

Туре	:	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

5. Toxicity		ld 95823-36-2
		Date 06.11.2006
GLP	: no	
Test substance		
Remark	 No significant toxic signs were obser period. All rats appeared normal up deaths occurred rats throughout the were made at necropsy. Route of administration: Inhalation Frequency of Treatment: Single 6-h Dose/Concentration Levels: Saturat concentration was 3.0 mg/L. Control group and Treatment: Group controls for the substances tested in examined grossly. 	ved during the 6-hour exposure to 5 days following exposure. No study and no significant observations our exposure ed vapors - the mean nominal ps of rats that served as common this study were sacrificed and
Result	: LC50 > 3.0 mg/L	
Test condition	An atmosphere of saturated vapors of bubbler system that contained the te vaporized at a flow rate of 27 L/min. compartments within the exposure of mortality and toxic effects at 30-minu thereafter. The animals were observe at which point animals were sacrifice died during the exposure or observation	was produced by forcing air through a st substance. 31 ml of liquid was Animals were caged in wire mesh hamber. Animals were observed for ite intervals during exposure and daily ed for two weeks following exposure, ad and necropsied. Any animals that tion periods were necropsied.
Test substance	CAS No. 95823-36-2; Carboxylic aci	ds, C6-8-neo
Conclusion	: Under conditions of this study, Carbo	oxylic acid, C6-8 neo
Reliability	 (2) valid with restrictions No vapor concentration verification (a) 	analytical), study conducted pre-GLP.
Flag 27.09.2006	Critical study for SIDS endpoint	(6)
Туре	LC50	
Value	: > 3 mg/l	
Species	mouse	
Strain	other: Albino	
Sex	male	
Number of animals	10	
Venicie	other: none	
Exposure time	e 6 hour(s)	
Method	other: NA	
Year	1964	
GLP	no	
Test substance	:	
Remark	 No significant toxic signs were obser period. All mice appeared normal up the mice developed uticaria. No deat study and no significant observations Route of administration: Inhalation Frequency of Treatment: Single 6-hr Dose/Concentration Levels: Saturat concentration was 3.0 mg/L. Control group and Treatment: Group controls for the substances tested in examined grossly. 	ved during the 6-hour exposure to 5 days following exposure, when ths occurred in mice throughout the s were made at necropsy. our exposure ed vapors - the mean nominal ps of mice that served as common this study were sacrificed and
Result Test condition	 LC50 > 3.0 mg/L An atmosphere of saturated vapors values bubbler system that contained the tervaporized at a flow rate of 27 L/min. compartments within the exposure climortality and toxic effects at 30-minute 	was produced by forcing air through a st substance. 31 ml of liquid was Animals were caged in wire mesh hamber. Animals were observed for ute intervals during exposure and daily

5. Toxicity	ld 95823-36-2 Date 06.11.2006	
Test substance Conclusion Reliability Flag 27.09.2006	 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. CAS No. 95823-36-2; Carboxylic acids, C6-8-neo Under conditions of this study, Carboxylic acid, C6-8 neo has a low order of acute inhalation toxicity in mice. (2) valid with restrictions No vapor concentration verification (analytical), study performed pre-GLP. Critical study for SIDS endpoint 	
5.1.3 ACUTE DERMAL	ΤΟΧΙCΙΤΥ	
Value Species Strain Sex Number of animals Vehicle Doses Method Year GLP Test substance	 > 3160 mg/kg bw rabbit other: Albino male/female 4 other: none other 1964 no 	
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.	
Result Test condition	 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 LD50 > 3160 mg/kg Undiluted test sample was applied to clipped, intact abdominal skin under 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 o 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 percention. 	

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

5. Toxicity	ld 95823-36-2 Date 06.11.2006
Flag 27.09.2006	Study performed Pre-GLP. : Critical study for SIDS endpoint (6)
5.1.4 ACUTE TOXICITY,	THER ROUTES
5.2.1 SKIN IRRITATION	
Species Concentration Exposure Exposure time Number of animals Vehicle PDII Result Classification Method Year GLP	 rabbit Semiocclusive 24 hour(s) 1964 no
Test substance	:
	 Dose/Concentration Levels. 30, 200, 734, 5100 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.

b. I OXICITY	Date 06.11.2006	
Test substance Reliability	 CAS No. 95823-36-2; Carboxylic acids, C6-8-neo (2) valid with restrictions Study performed Bro CLP 	
Flag 27.09.2006	: Critical study for SIDS endpoint	(
5.2.2 EYE IRRITATION		
Species	: rabbit	
Concentration Dose		
Exposure time	: . not rinsed	
Number of animals	: 6	
Result		
Classification		
Year	: 1964	
GLP Tost substance	: 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. S iritis was seen in all rabbits disappearing within 48 hours. Dullness an corneal opacity with apparent sloughing and vascularisation were obsein all animals, but these reactions disappeared by the fourth and sever days in four of the six rabbits.	Sligh d erve nth
lest condition	food and water.	ate
	The test material was administered as a single instillation of 0.1 ml into lower conjunctival sac of the left eye of each animal. The upper and lo lids were gently held together for approximately 1 second to prevent lo the material. The contralateral eye served as the control.	o the owe oss o
Toot outpotonics	The eyes of each animal were examined 24, 48, and 72 hours, and 4, and 10 days after administration. At each interval the treated and con eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale.	7 trol
Reliability	: (2) valid with restrictions Study performed Pre-GLP.	
Flag	: Critical study for SIDS endpoint	
21.09.2006		(

5.4 REPEATED DOSE TOXICITY

rabbit
male
other: Albino
dermal
10 applications with a two-day rest between the 5th and 6th applications.

5. Toxicity		ld 95823-36-2 Date 06.11.2006
Post exposure period Doses Control group NOAEL Method Year GLP Test substance	55.4 mg/kg, 553.7 mg/kg other: Isopropyl Alcohol (IPA) was administered to 2.5 ml/kg body weight per application. = 553.7 mg/kg other 1964 no	o 8 animals at a level of
Remark	Animals in the low dose group showed normal app throughout the study. With the exception of one a slight weight loss, the animals in the low dose group body weight gain. In the high dose group, 3 of the normal appearance and behavior and either maint a slight weight loss. From the fifth through the nim- animal had labored breathing, weight loss, and wa after the final application. Upon necropsy, this ani emphysematous lungs in addition to hemorrhagic medulla. The death of this animal was deemed to treatment. Gross pathology of the remaining anim group did not reveal any abnormalities other than a in the liver of one of the rabbits. Repeat application histopathological alterations to the liver or kidney of third application and lasted through the study. At the moderate erythema was observed and slight to mo- present from the second through the fifth application application, moderate to marked atonia, desquare was observed through the remainder of the study. areas of necrosis at the application site and in two hypersensitive to touch. No. of animals/sex/dose: 4/dose Vehicle: None	earance behavior nimal that showed a up showed an overall 4 animals displayed ained their weight or had th application, the fourth s found dead 24 hours mal had congested and areas in the renal be unrelated to the als of the high dose a slight parasitic infection ns did not cause any of the rabbits. Erved during the first ation that followed the he highest dose, slight to oderate edema was ons. After the fourth ation, and slight fissuring All animals showed animals, the skin was
Result	Statistical method: Not reported For systemic effects: NOAEL = 553.7 mg/kg Carboxylic acid, C6-8 neo produced moderate to s	evere skin irritation.
Test condition	The test material was applied to clipped abdomina binder or a collar was used to prevent ingestion of Animals were housed individually and allowed free water. Each animal was weighed, sacrificed, and after the final application of test material. At the be prior to the final application, the following clinical p evaluated: total erythrocyte count, total and differe hematocrit, and urinalysis. Histological analysis w sections of liver and kidney. Sections of brain, thy kidneys, adrenals, skin, and bone marrow were pro- future analysis.	I skin. A loose gauze the test substance. access to food and necropsied 24 hours eginning of the study and arameters were ntial leukocyte count, as performed on roid, lungs, heart, liver, eserved for possible
Test substance Conclusion	CAS No. 95823-36-2; Carboxylic acids, C6-8-neo Under the conditions of this study, Carboxylic acid has a low order or systemic toxicity following repea	, C6-8 neo ated dermal exposure.
Reliability	(2) valid with restrictions Study performed Pre-GLP.	· · · · · · · · · · · · · · · · · · ·
27.09.2006		(15)

5.5 GENETIC TOXICITY 'IN VITRO'

5. Toxicity

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type Species Sex Strain Route of admin. Exposure period Frequency of treatm. Premating exposure per Male Female Duration of test	iod	One generation study rat male/female Sprague-Dawley other: Dietary
No. of generation studies Doses Control group Method Year GLP Test substance		0, 1000, 5000, 7500, and 10,000 ppm in diet other: 10/sex other 1999 yes 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 Test condition	:	Maternal and Offspring NOAEL = 7500 ppm 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

5. Toxicity	ld 95823-36-2 Date 06.11.2006
	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 Conclusion	 Isooctanoic Acid (CAS No. 25103-52-0) 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 Flag 27.09.2006	: (1) valid without restriction : Critical study for SIDS endpoint (13)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species Sex Strain Route of admin. Exposure period Frequency of treatm. Duration of test Doses Control group NOAEL maternal tox. Method Year GLP Test substance	 rat female Sprague-Dawley other: oral gavage Days 6-15 of gestation 0, 50, 250, 600, or 800 mg/kg other: Controls received 800 mg/kg of distilled water = 250 mg/kg bw OECD Guide-line 414 "Teratogenicity" 1986 yes
Remark Result	 Number/sex/dose: 22/dose Statistical methods: ANOVA, Kruskal-Wallis, Fisher's exact test 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
	20 / 20

5. Toxicity	ld 95823-36-2
2	Date 06.11.2006
	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.
Test condition	 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. 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 examined.
Test substance	ossification variations.
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
27.09.2006	. Childai study for SiDS enupoint (8)
Species	· rat
Sex	: female
Strain	: Sprague-Dawley
Route of admin.	conter: 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 Year	- 1995
GLP	: Ves
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 30 / 36

5. Toxicity	ld 95823-36-2 Date 06.11.2006	
	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.	
Test condition	 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. 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 	5
Test substance	 determine sex and for gross malformations. Isooctanoic Acid (CAS No. 25103-52-0) Under the conditions of this study, lease tancia acid is not a collective. 	
Conclusion	developmental toxicant.	
Reliability	: (2) valid with restrictions	
27.09.2006	(12) was performed as a range-infulling study.)

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. Eff. Against Target Org. and Intended Uses

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

9. Refere	Id 95823-36-2 Date 06.11.2006
(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



2006 NOV 14 AM 10: 55

IUCLID

Data Set

Existing Chemical CAS No. EINECS Name EC No. Molecular Weight Molecular Formula	 ID: 26896-20-8 26896-20-8 Neodecanoic acid 248-093-9 173 C10H20O2
Producer related part Company Creation date	: ExxonMobil Biomedical Sciences Inc. : 18.09.2001
Substance related part Company Creation date	: ExxonMobil Biomedical Sciences Inc. : 18.09.2001
Status Memo	: : ExxonMobil Chemical Company (EMCC) Neoacids - HPV
Printing date Revision date Date of last update	: 06.11.2006 : : 19.10.2006
Chapter (profile) Reliability (profile) Flags (profile)	 Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 Reliability: without reliability, 1, 2, 3, 4 Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

.

1. General Information

ld 26896-20-8 Date 06.11.2006

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

ee	tree	text
	ee	ee tree

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	:	

I. General Informa	tion	Id 26896-20-8 Date 06.11.2006
Colour Odour	:	
Remark	: CAS Registry Number, Name, an Neoacids C5 to C28 Category and	d General Structure for Members of the data Analogue Substances:
29.09.2006	CAS RN: 26896-20-8 TSCA Name: Neodecanoic acid- R length (C number): C10 Structure of R: Linear Category Member: Yes	
1.1.2 SPECTRA		
1.2 SYNONYMS AND	TRADENAMES	
2 2-Dimethyloctanoic a	cid	
19 11 2001		
Neodecanoic Acid 10		
29.09.2006		
29.09.2000		
1.3 IMPURITIES		
Purity CAS-No EC-No EINECS-Name Molecular formula Value	 typical for marketed substance 26896-20-8 248-093-9 neodecanoic acid C10H20O2 > 97 % w/w 	
29.09.2006		
1.4 ADDITIVES		
Purity type CAS-No EC-No EINECS-Name Molecular formula Value Function of additive	 typical for marketed substance 26896-20-8 248-093-9 neodecanoic acid . 	
Remark 29.09.2006	: No additives present	

1. General Information	ld 26896-20-8
	Date 06.11.2006
1.6.1 LABELLING	
1.6.2 CLASSIFICATION	
1.6.3 PACKAGING	
1.7 USE PATTERN	
Type of use: industrialCategory: Chemical industry: used in s	synthesis
Remark : Primarily used as an interme	ediate in the production of drying agents, PVC
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	
184 MAJOR ACCIDENT HAZARDS	
1.8.5 AIR POLLUTION	
1.8.0 LISTINGS E.G. CHEMICAL INVENTORIES	
1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS	
1.9.2 COMPONENTS	

1. General	Information	ld Date	26896-20-8 06.11.2006
1.10 SOUR	CE OF EXPOSURE		
1.11 ADDIT	IONAL REMARKS		
1.12 LAST I	LITERATURE SEARCH		
1.13 REVIE	WS		

2.1 MELTING POINT

Value Sublimation Method Year GLP Test substance	: = 57.1 °C : : other: ASTM D97 : 2003 : no data :
Test substance Reliability	 CAS No. 26896-20-8; Neodecanoic acid (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 29.09.2006	: Critical study for SIDS endpoint (11)
2.2 BOILING POINT	
Value Decomposition Method Year GLP Test substance	: = 250 - 257 °C at : : other: D1078/01 : 2003 : no data :
Test substance Reliability Flag 29.09.2006	 CAS No. 26896-20-8; Neodecanoic acid (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. Critical study for SIDS endpoint
2.3 DENSITY	
Type Value Method Year GLP Test substance	: density : = .91 at 20 °C : : 2003 : no data :
Test substance Reliability	 CAS No. 26896-20-8; Neodecanoic acid (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 29.09.2006	: Critical study for SIDS endpoint (11)

2.3.1 GRANULOMETRY

2. Physico-Chemical Data

(6)

2.4 VAPOUR PRESSURE

Value Decomposition Method Year GLP Test substance	: : : : : : : : : : : : : : : : : : : :	= .009 hPa at 25 °C other (calculated) 2003
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 29.09.2006	:	Critical study for SIDS endpoint

2.5 PARTITION COEFFICIENT

Partition coefficient Log pow pH value Method Year GLP Test substance	 octanol-water = 3.9 at 25 °C other (calculated) 2003
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.		
рКа	:	4.8 at 25 °C
Description	:	
Stable	:	
Deg. product	:	

2. Physico-Chemical Data

Method Year GLP Test substance	2003	
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	
Ē	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	
		16

2.7 FLASH POINT

Valu Typ Met Yea GLF Tes	ue e hod r b t substance	:	= 122 °C open cup other: COC ASTM D92 2003 no data	
Tes Reli	t substance ability	:	CAS No. 26896-20-8; Neodecanoic acid (2) valid with restrictions Although the original data were not retrieved and reviewed for quality, the were developed following acceptable test methods and therefore considered to be reliable.	эy
Flag 02.1) 0.2006	:	Critical study for SIDS endpoint (1	11)
2.8	AUTO FLAMMABILI	ITY		
2.9	FLAMMABILITY			
2.10	EXPLOSIVE PROPE	RT	IES	
2.11	OXIDIZING PROPER	RTIE	ES	
2.12	DISSOCIATION CO	NST	ANT	
Acie Met	d-base constant hod	:	4.8 other: calculated 8 / 39	

,		Date 06.11.2006
Year	: 2003	
GLP	:	
Test substance	:	
Method	: pKa calculation by SPARC 2003 usi	ing a Linux calculation engine.
Remark	: SPARC On-line calculator can be ac	ccessed at
	http://ibmlc2.chem.uga.edu/sparc/in-	dex.cfm
Test substance	: CAS No. 26896-20-8; Neodecanoic	acid
Reliability	: (2) valid with restrictions	
	The value was calculated based on SPARC. This robust summary has	the chemical structure as modeled by a reliability rating of 2 because the dat
	are calculated and not measured.	, , ,
02.10.2006		(1
Value	• - 40 - et 20 °C	
value	= 40 - at 20 °C	
Result	- other: ASTM D445	
Voor	• 2003	
GIP	no data	
Test substance		
	•	
Damarla	: Value measured in cSt	
Remark		
Remark Test substance	: CAS No. 26896-20-8; Neodecanoic	acid
Remark Test substance Reliability	CAS No. 26896-20-8; Neodecanoic(2) valid with restrictions	acid
Remark Test substance Reliability	 CAS No. 26896-20-8; Neodecanoic (2) valid with restrictions Although the original data were not r were developed following acceptable considered reliable 	acid retrieved and reviewed for quality, the e test methods and therefore
Remark Test substance Reliability	 CAS No. 26896-20-8; Neodecanoic (2) valid with restrictions Although the original data were not a were developed following acceptable considered reliable. 	acid retrieved and reviewed for quality, the e test methods and therefore

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Туре	:	air
Light source	:	Sun light
Light spectrum	÷	nm based en intensity of symbolisht
	•	based on intensity of sunlight
Sensitizer		ОН
Conc. of sensitizer	÷	1500000 molecule/cm ³
Rate constant	:	= .00000000075357 cm ³ /(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* OH- Rate Constant half-life (days) (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.
Test condition	:	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. Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.
		Temperature: 25°C
		10/30

ld 26896-20-8 Date 06.11.2006

Test substance Reliability Flag 02.10.2006	 Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3 CAS No. 26896-20-8; Neodecanoic acid (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. Critical study for SIDS endpoint (6)
Type Light source Light spectrum Relative intensity Deg. product Method Year GLP Test substance	water nm based on intensity of sunlight other (calculated): Technical discussion
Remark Result	 These data represent a key study for characterizing the potential of substances in the Neoacids C5 to C28 Category to undergo direct photodegradation. 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

3. Environmental I	ate and Pathways	ld 26896-20-8 Date 06.11.2006
	Property Estimation Methods, Mco USA.	Graw-Hill Book Company, New York,
	Zepp, R. G. and D. M. Cline. 1977 Aqueous Environment, Environ. S	 Rates of Direct Photolysis in the ci. Technol., 11:359-366.
Test substance Flag 01.09.2006	 Boethling, R.S., Mackay, D. 2000. Methods for Chemicals, CRC Pres Neoacids C5 to C28 Category me Critical study for SIDS endpoint 	Handbook of Property Estimation ss, Boca Raton, FL, USA. mbers (5)
3.1.2 STABILITY IN WA	TER	
Type t1/2 pH4 t1/2 pH7 t1/2 pH9 Deg. product Method Year GLP Test substance	: abiotic : at °C : at °C : at °C : : other: technical discussion :	
Remark Result	 These data represent a key study substances in the Neoacids C5 to Hydrolysis as a Function of Molec 	for characterising the potential of C28 Category to undergo hydrolysis. ular Structure
	Hydrolysis of an organic molecule with water (H2O) to form a new ca bond is cleaved (Gould, 1959; Ha is referred to as a nucleophilic sub group being replaced by the incon molecule.	occurs when a molecule (R-X) reacts arbon-oxygen bond after the carbon-X rris, 1982). Mechanistically, this reaction ostitution reaction, where X is the leaving ning nucleophilic oxygen from the water
	Chemicals that are susecptible to can be displaced by a nucleophilic have a potential to hydrolyze inclu carboxylic acid esters and lactone sulfonic acid esters (Neely, 1985). renders a compound resistant to h	hydrolysis contain functional groups that substitution reaction. Substances that de alkyl halides, amides, carbamates, s, epoxides, phosphate esters, and The lack of a suitable leaving group hydrolysis.
	Aliphatic acids are resistant to hyc group that is hydrolytically reactive	Irolysis because they lack a functional e (Harris, 1982).
	References:	
	Gould, E.S. (1959), Mechanism ar Reinhart and Winston, New York,	nd Structure in Organic Chemistry, Holt, NY, USA.
	Harris, J.C. (1982), "Rate of Hydro Reehl, and D.H. Rosenblatt, eds., Estimation Methods, McGraw-Hill	olysis," Chapter 7 in: W.J. Lyman, W.F. Handbook of Chemical Property Book Company, New York, NY, USA.
Test substance Conclusion	 Neely, W. B. 1985. Hydrolysis. In: Environmental Exposure from Che Boca Raton, FL, USA. Neoacids C5 to C28 Category me Hydrolysis will not contribute to the environment. 	W. B. Neely and G. E. Blau, eds. emicals. Vol I., pp. 157-173. CRC Press, mbers e removal of neoacids from the

Flag 01.09.2006 : Critical study for SIDS endpoint (4 3.1.3 STABILITY IN SOL (4 3.2.1 MONITORING DATA (4 3.2.2 FIELD STUDIES (4 3.1.3 STABILITY IN SOL (4 3.2.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS (4 3.2.2 FIELD STUDIES (5) 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS (5) Ype : fugacity model level II Media : Other: air - sediment(5) - soil - water Air : % (Fugacity Model Level II) Soil : % (Fugacity Model Level III) Biota : % (Fugacity Model Level IIIII) Soil : % (Fugacity Model Level IIIII) Method : Other: Calculation according Mackay, Level III Ymethod : 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 II Yugacity allows non-equilation model new consected media as steady state, and illustrate important transport and transformation or necesses. Physicochemical input values for the model were calculated using the EPWIN tatimation values used: Molecular masses 172.27 g/mol Water resultility = 60 mg/L Water resultility = 60 mg/L Vapour pressure = 0.55 Pa Pa Pa <t< th=""><th>3. Environmental Fa</th><th>ate and Pathways</th><th>ld Date</th><th>26896-20-8 06.11.2006</th></t<>	3. Environmental Fa	ate and Pathways	ld Date	26896-20-8 06.11.2006
 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) Soil : % (Fugacity Model Level I) Soil : % (Fugacity Model Level I) Soil : % (Fugacity Model Level I) Biota : % (Fugacity Model Level I) Soil : % (Fugacity Model Level I) Soil : % (Fugacity Model Level I) Biota : % (Fugacity Model Level I) Soil : % (Fugacity Model Level I) Soil : % (Fugacity Model Level I) Biota : % (Fugacity Model Level IIII) Year : 2003 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 teady state, and illustrate important transport and transformation processes. Physicochemical input values for the model were calculate using the PUWIN Estates and values were also used where available and obtained from the EPUWIN database. Distinution data from the equilibrium model provide basic informatial partitioning behavior of chemicals between selected environmental compartments (Le. air, water, soil, and sediment). Input values used: Model calculation according Mater available and obtained from the EPUWIN database. Distinution and provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (Le. air, water, soil, and sediment). Input values used: Model calculation according Mater available and obtained from the EPUWIN database. Distincuton and transformatic partitioning behavior of chemicals	Flag 01.09.2006	: Critical study for SIDS endpoint		(4)
3.2.1 MONITORING DATA 3.2.2 FIELD STUDIES 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS Type : fugacity model level II 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 I) Biota : % (Fugacity Model Level I) Biota : % (Fugacity Model Level I) Bota : % (Fugacity Model Level I) Bota : % (Fugacity Model Level I) 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 value 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	3.1.3 STABILITY IN SOIL			
 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) Soil :: % (Fugacity Model Level I) Soil :: % (Fugacity Model Level I) Soil :: % (Fugacity Model Level I) Biota :: % (Fugacity Model Level I) 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 EPIVIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIVIN 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 = 99 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 - 72.3% Yeater = 66.7% Soil - 57.7% Test substance : CAS No. 26896-20-8; Neodecanoic acid 	3.2.1 MONITORING DAT	A		
3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS Type : fugacity model level III Media : : other: air - sediment(s) - soil - water Air : : (Fugacity Model Level I) Soil : : % (Fugacity Model Level I) Biota : % (Fugacity Model Level I) Biota : % (Fugacity Model Level I) Biota : % (Fugacity Model Level I) Soil : : % (Fugacity Model Level I) Biota : : : : Year : : : : Year : : : : : Method : : : : : : 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 - 240000 hrs : :	3.2.2 FIELD STUDIES			
Type : fugacity model level III Media : other: air - sediment(s) - soil - water Air : % (Fugacity Model Level I) Soil : % (Fugacity Model Level I) Biota : % (Fugacity Model Level I) Biota : % (Fugacity Model Level I/III) Biota : % (Fugacity Model Level I/III) Method : other: Calculation according Mackay, Level III Year : 2003 Method : other: Calculation according Mackay, Level III Year : 2003 Method : other: Calculation according Mackay, Level III Year : 2003 Method : other: Calculation according Mackay, Level III Year : 2003 Method : other: Calculation according Mackay, Level III Year : 2003 Method : other: Calculation according Mackay, Level III Year : 2003 Method : other: Calculation according Mackay, Level III Year : 2003 Method : other: Calculation according Mackay, Level III Year : 2003 Method : other: Calculation according Mackay indication according Mac	3.3.1 TRANSPORT BETW	EEN ENVIRONMENTAL COMPARTMEN	ITS	
Result : Air - 0.28% Water - 66.7% Soil - 5.7% Sediment - 27.3% Sediment - 27.3% Test substance : CAS No. 26896-20-8; Neodecanoic acid	Type Media Air Water Soil Biota Soil Method Year Method	 fugacity model level III other: air - sediment(s) - soil - water % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I)/III) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) other: Calculation according Mackay, 2003 The EQC Level III model is a steady sedetermining how the medium of release III fugacity allows non-equilibrium commedia as steady state, and illustrate in processes. Physicochemical input values for the released where available and obtained from data from the equilibrium model provide partitioning behavior of chemicals beth compartments (i.e., air, water, soil, and 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 - 720000 hrs 	Level III state model that is se affects environ iditions to exist be mportant transpor model were calcu Measured input va om the EPIWIN da de basic informati ween selected en ad sediment).	s useful for mental fate. Level tween connected t and transformation lated using the alues were also atabase. Distribution on on the potential vironmental
Soll - 5.7%Sediment - 27.3%Test substance:CAS No. 26896-20-8; Neodecanoic acid	Result	: Air - 0.28% Water - 66.7%	,	
	Test substance	Soll - 5.7% Sediment - 27.3% : CAS No. 26896-20-8; Neodecanoic a	cid	

Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag 02 10 2006	:	Critical study for SIDS endpoint (15)
Type Media Air Water Soil Biota Soil Method Year		fugacity model level I other: air - biota - sediment(s) - soil - water % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) other: Calculation according Mackay, Level I 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
Result	:	Vapour pressure = 0.93 Pa log Kow = 3.9 Melting point = 57.1 deg C Soil - 81.1% Air - 5.5%
Test substance	-	Water - 11.5% Sediment - 1.8% Suspended Sed - 0.06% Biota - <0.01% CAS No. 26896-20-8: Neodecapoic 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.
Reliability	:	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. (2) valid with restrictions
		calculated and not measured.
над 02.10.2006	:	Critical study for SIDS endpoint (15)
3. Environmental Fate and Pathways

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 **BIODEGRADATION**

Type Inoculum Contact time Degradation Result Deg. product Method Year GLP Test substance	 aerobic activated sludge, domestic 28 day(s) = 11 (±) % after 28 day(s) OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test" 1996 yes
Remark Result	 Test Type: Manometric Respirometry Test 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.
	% Degradation* Mean % Degradation Sample (day 28) (day 28) Test Material 20.5, 3.60, 8.90 11.0 Na Benzoate 98.9, 95.5 97.2
Test condition	 replicate data 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. Environmental Fate and Pathways

3.7 BIOACCUMULATION

BCF Elimination Method Year GLP Test substance		= 3.16 other: calculated 2003
Method	:	Calculated values using BCFWIN version 2.13, a subroutine of the
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
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 02.10.2006	:	Critical study for SIDS endpoint (6)

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type Species Exposure period Unit LC50 Limit test Analytical monitoring Method Year GLP Test substance	 semistatic Oncorhynchus mykiss (Fish, fresh water) 96 hour(s) mg/l = 37.2 measured/nominal no yes OECD Guide-line 203 "Fish, Acute Toxicity Test" 1996 yes
Remark Result	 Statistical Method: Bionomial Method 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.
Test condition	Nominal Conc.Measured Conc.Mortality @ 96 hr.ControlBelow detection06.25 mg/L10.3 mg/L012.5 mg/L13.6 mg/L025 mg/L26.3 mg/L050 mg/L52.5 mg/L0100 mg/L102 mg/L01Individual 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 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.
Test substance Conclusion Reliability Flag 29.09.2006	 Fish Mean Wt.= 0.260g. Mean Total length = 3.3cm, Test Loading = 0.29 g of fish/L. CAS No. 26896-20-8; Neodecanoic acid Test substance is considered moderate toxicity. (1) valid without restriction Critical study for SIDS endpoint (9)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4. Ecotoxicity

ld 26896-20-8 Date 06.11.2006

Type Species Exposure period Unit LL50 Analytical monitoring Method Year GLP Test substance	 static Daphnia magna (Crustacea) 48 hour(s) mg/l = 47.1 no other: USEPA -660/3-75-009 Methods for Acute Toxicity with Fish and Macroinvertebrates, and Amphibians, 1975 1977 no
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 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
Tost substance	Organisms were <24 hrs old, supplied by in-house cultures.
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. Ec	cotoxicity Dat	d 26896-20-8 e 06.11.2006
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. Toxicity

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type Value Species Strain Sex Number of animals Vehicle Doses Method Year GLP Test substance		LD50 = 2000 mg/kg bw rat Sprague-Dawley male 5 other: none 34.6, 120, 417, 1450, 5000, and 10000 mg/kg other 1964 no
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
Flag		Critical study for SIDS endpoint
04.10.2006	•	(7)

5.1.2 ACUTE INHALATION TOXICITY

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

5. Toxicity	ld 26896-20-8 Date 06.11.2006
Doses Exposure time Method Year GLP Test substance	: 6 hour(s) : other : 1964 : no
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 Test condition	 LC50 > 3.0 mg/L 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 Conclusion Reliability	 CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid) Under conditions of this study, 2,2-Dimethyloctanoic acid has a low order of acute inhalation toxicity in mice and rats. (2) valid with restrictions
16.10.2006	No vapor concentration verification (analytical) (7)
Type Value Species Strain Sex Number of animals Vehicle Doses Exposure time Method Year GLP Test substance	 LC50 > 511 mg/m³ rat Wistar male/female 20 other: None 6 hour(s) other 1982 no
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

5. Toxicity	ld 26896-20-8
2	Date 06.11.2006
	normal except for a slight weight loss on the first and second post- exposure days in both the control and treated groups (all species).
Result Test condition	 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 LC50 > 511 mg/m3 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
Test substance	 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. CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid) Under conditions of this study, acrosolized 2.2 Dimethyloctanoic acid.
Reliability	 bilder conditions of this study, aerosolized 2,2-Dimentification activity has a low order of acute inhalation toxicity in mice, rats, and guinea pigs. (1) valid without restriction
Flag 04.10.2006	: Critical study for SIDS endpoint (1)
Type Value Species Strain Sex Number of animals Vabiale	: LC50 : > 3 mg/l : mouse : other: Swiss albino : male : 10
Doses Exposure time	: 6 hour(s)
Method Year	: other : 1964
GLP Test substance	: no
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.
	22 / 39

5. Toxicity	ld 26896-20-8
er rekienty	Date 06.11.2006
Result Test condition	 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. LC50 > 3.0 mg/L 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 pecropsied.
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 Value	: LC50 : > 511 mg/m ³
Species	: mouse
Strain	: other: Swiss albino
Sex	: male/female
Number of animals	: 20
Venicie	: otner: None
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 23 / 39

5. Toxicity	ld 26896-20-8 Date 06.11.2006	
	Control group and Treatment: 10/sex/species	
Result Test condition	LC50 > 511 mg/m3 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 Conclusion	CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid) 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 Flag 04.10.2006	(1) valid without restriction Critical study for SIDS endpoint (1)	
Type Value Species Strain Sex Number of animals Vehicle Doses Exposure time Method Year GLP Test substance	LC50 > 511 mg/m ³ guinea pig Hartley male/female 20 other: None 6 hour(s) other 1982 no	
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	

o. Toxicity	Date 06.11.2006
Result Test condition	 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 LC50 > 511 mg/m3 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 sacrifice 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 the died or were sacrificed during the study. Major organs were examined for macroscopic abnormalities and 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

Туре	: 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 applicate of elight to mederate ar thema which

5. Toxicity	ld 26896-20-8 Date 06.11.2006
Result Test condition	 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 LD50 > 3160 mg/kg 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	acute dermal toxicity in rabbits.
Reliability	: (2) valid with restrictions
Flog	Study Performed Pre-GLP
гад 16.10.2006	. Chica study for SIDS enupoint (7)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

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

5. Toxicity	ld 26896-20-8 Date 06.11.2006
	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.
Result	After the Day 7 observation, all animals were sacrificed without further examination.
iteoun	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.
Test substance Reliability Flag 04.10.2006	 Based on these finding the primary iiritation index was 0.67, which indicates the test substance is a mild irritant to rabbit skin. CAS No. 26896-20-8; Neodecanoic acid (1) valid without restriction Critical study for SIDS endpoint
Species Concentration Exposure Exposure time Number of animals Vehicle PDII Result Classification Method Year GLP	: rabbit : : Semiocclusive : 24 hour(s) : 8 : : : : : : : : : : : : :
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.
Test condition	 Route of administration: Dermal Frequency of Treatment: Single Dose Dose/Concentration Levels: 50, 200, 794, 3160 mg/kg Control group and Treatment: None 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 27 / 39

Test substance:Reliability:16.10.20062.2 EYE IRRITATIONSpecies:Concentration:Dose:Exposure time:Comment:Number of animals:Vehicle:Result:Classification:Method:Year:GLP:Test substance:Remark:	were weighed, sacrificed, and necropsied. CAS No. 26896-20-8; Neodecanoic acid (2) valid with restrictions Study Performed Pre-GLP (7 rabbit undiluted not rinsed 6
16.10.2006SpeciesConcentrationDoseExposure timeCommentNumber of animalsVehicleResultClassificationMethodYearGLPTest substanceRemark	rabbit undiluted not rinsed 6
Species : Concentration : Dose : Exposure time : Comment : Number of animals : Vehicle : Result : Classification : Method : Year : GLP : Test substance : Remark :	rabbit undiluted not rinsed 6
Species:Concentration:Dose:Exposure time:Comment:Number of animals:Vehicle:Result:Classification:Method:Year:GLP:Test substance:Remark:	rabbit undiluted not rinsed 6
Species:Concentration:Dose:Exposure time:Comment:Number of animals:Vehicle:Result:Classification:Method:Year:GLP:Test substance:Remark:	rabbit undiluted not rinsed 6
Concentration:Dose:Exposure time:Comment:Number of animals:Vehicle:Result:Classification:Method:Year:GLP:Test substance:Remark:	undiluted not rinsed 6
Dose:Exposure time:Comment:Number of animals:Vehicle:Result:Classification:Method:Year:GLP:Test substance:Remark:	not rinsed 6
Exposure time:Comment:Number of animals:Vehicle:Result:Classification:Method:Year:GLP:Test substance:Remark:	not rinsed 6
Comment:Number of animals:Vehicle:Result:Classification:Method:Year:GLP:Test substance:Remark:	not rinsed 6
Number of animals:Vehicle:Result:Classification:Method:Year:GLP:Test substance:Remark:	6
Vehicle:Result:Classification:Method:Year:GLP:Test substance:Remark:	
Result:Classification:Method:Year:GLP:Test substance:Remark:	none
Classification:Method:Year:GLP:Test substance:Remark:	
Method:Year:GLP:Test substance:Remark:	
rear:GLP:Test substance:Remark:	1001
GLF.Test substance:Remark:	1964
Remark :	10
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.
Test substance :	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. 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	(

5.4 REPEATED DOSE TOXICITY

Туре	:	
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

5. Toxicity	ld 26896-20-8 Date 06.11.2006
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.
Test condition	 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. 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, the following clinical parameters were evaluated: total erythrocyte count, total and differential leukocyte count, hematocrit, and urinalysis. Histological analysis was performed on
Test substance	 kidneys, adrenals, skin, and bone marrow were preserved for possible future analysis. CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid) Under the conditions of this study. 2 2-Dimethyloctanoic acid has a low.
Reliability	 order of systemic toxicity following subchronic dermal exposure. (2) valid with restrictions
	Study performed Pre-GLP.
Flag	: Critical study for SIDS endpoint (10)
04.10.2000	(12)

5.5 GENETIC TOXICITY 'IN VITRO'

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

ld 26896-20-8 Date 06.11.2006

5. Toxicity

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 his increase in the number of revertant colonies of all tested Salmo in the presence or absence of S9 mix after application. Positiv gave the expected increase in the number of histidine+ reverta presence as well as in the absence of S9 mix. 	igher onella strains ve controls ants in the
Test substance	: CAS No. 26896-20-8; Neodecanoic acid	
Conclusion	: Neodecanoic acid is not mutagenic in strains of the bacteria S. under conditions of this assay.	. typhimurium
Reliability	: (2) valid with restrictions Although the original data was not retrieved and reviewed for or were developed following acceptable test methods and therefore	quality, they pre
Flag	: Critical study for SIDS endpoint	
19.10.2006		(16)
Туре	: 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 Test substance		
	-	
Remark	 Two independent tests were conducted, both in the presence a of S9 mix. Cells were exposed to neodecanoic acid for 24 or 4 The cultures were processed for chromosomal aberrations. A r inhibition was calculated. 	and absence 18 hours. mitotic index
	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 cells with chromosomal aberrations at each concentration or the tested, with or without metabolic activation. Positive control su (mitomycin C and cyclophosphamide) confirmed the activity ar of the test system.	the % of me point lbstances nd sensitivity
Test substance	: CAS No. 26896-20-8; Neodecanoic acid	
Conclusion	: Neodecanoic acid is not genotoxic in human lymphocytes in vir conditions of this assay.	tro under
Reliability	 (2) valid with restrictions Although the original data was not retrieved and reviewed for c were developed following acceptable test methods and therefore 	quality, they pre
	considered reliable.	

5. Toxicity

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

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

5. Toxicity	ld 26896-20-8
	Date 06.11.2006
	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 Conclusion	 Analog substance: Isononanoic Acid (CAS No. 3302-10-1) Under the conditions of this study the test substance did not adversely affect reproductive parameters at deses that were penterie to the dams or
Reliability	their offspring.(1) valid without restriction
Flag 04.10.2006	: Critical study for SIDS endpoint (10)
Type Species Sex Strain Route of admin. Exposure period	 other: Three Generation rat male/female Sprague-Dawley other: Dietary
Frequency of treatm. Premating exposure per	: Continuous od
Male Female	: P1: 9 weeks : P1: 9 weeks
Duration of test No. of generation	: 3 generations
studies Doses Control group NOAEL parental NOAEL F1 offspring NOAEL F2 offspring Method Year GLP	 0, 100, 500, 1500 ppm in diet other: 0, 100, 500, 1500 ppm in diet = 1500 ppm = 1500 ppm = 1500 - ppm other 1968 no
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

5. Toxicity	ld 26896-20-8
_	Date 06.11.2006
Result	 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 NOAEL Parental: 1500 ppm NOAEL F1 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 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.
Test substance Conclusion Reliability	 One week following the weaning of the F1A litters, the P1 parents were remated 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. CAS No. 26896-20-8; Neodecanoic acid (2,2-dimethyloctanoic acid) Under the conditions of this study, dietary exposure to 2,2-Dimethyloctanoic acid has a low order of reproductive toxicity in rats. (2) valid with restrictions
04.10.2006	Study performed pre-GLP (13)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5. To	xicity	ld ate	26896-20-8 06.11.2006	
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. Eff. Against	Target Org. and Intended Uses	
-----------------	-------------------------------	--

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

9. Referei	Id 26896-20-8 Date 06.11.2006
(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



2006 NOV 14 AM 10: 55

IUCLID

Data Set

Existing Chemical CAS No. EINECS Name EC No. TSCA Name	 ID: 68938-07-8 68938-07-8 Fatty acids, C9-13-neo- 273-114-3 Fatty acids, C9-13-neo-
Producer related part Company Creation date	: ExxonMobil Biomedical Sciences Inc. : 18.09.2001
Substance related part Company Creation date	: ExxonMobil Biomedical Sciences Inc. : 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) Reliability (profile) Flags (profile)	 Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 Reliability: without reliability, 1, 2, 3, 4 Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset Risk Assessment Directive 67/548/EEC, SIDS

1. General Information

ld 68938-07-8 Date 06.11.2006

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 : s	see free tex	٨t
-------------	--------------	----

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 Molecular weight Petrol class	::	C12H24O2 200.32
Flag 04.10.2006	:	Critical study for SIDS endpoint

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid

1. General Informa	ation Date 06.11.2006
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-
	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	= 99.0 % W/W
Remark	: The commercial product can be estimated at approximately 87% C9
	isomers and approximately 13% C13 isomers, with any remaining isome within the range indicated
04.10.2006	
1.4 ADDITIVES	
Purity type	: typical for marketed substance
CAS-No	: 68938-07-8
EC-NO	: 2/3-114-3 . Eatty acids C0 13 page
Molecular formula	- rany actus, US-10-1180- : C12H24O2
Value	
Function of additive	:
Remark	: No additives present
04.10.2006	· · · · · · · · · · · · · · · · · · ·
1.5 TOTAL QUANTITY	ſ
1.6.1 LABELLING	
0.2 CLASSIFICATION	

1. General Information

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use Category		:	industrial 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	1.7.1 DETAILED USE PATTERN				
1.7.2	2 METHODS OF MANUFACTURE				
		-			
1.8	REGULATORY MEASURES				
1.8.1	OCCUPATIONAL EX	(PC	OSURE LIMIT VALUES		
1.8.2	ACCEPTABLE RES	IDU	ES LEVELS		
1.8.3	3 WATER POLLUTION				
1.8.4	4 MAJOR ACCIDENT HAZARDS				
1.8.5	5 AIR POLLUTION				
1.8.6	3.6 LISTINGS E.G. CHEMICAL INVENTORIES				
1.9.1	1 DEGRADATION/TRANSFORMATION PRODUCTS				
102					
1.9.2	COMPONENTS				
1.10	SOURCE OF EXPOS	SUF	RE		
1 1 1		DV	e		
1.11					

1. General Information

ld 68938-07-8 Date 06.11.2006

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value Sublimation Method Year GLP Test substance	 = 37 - 76 °C other: ASTM D97 2003 no data
Test substance Reliability	 CAS No. 68938-07-8; Fatty acids, C9-13-neo- (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 12.10.2006	: Critical study for SIDS endpoint (9)
2.2 BOILING POINT	
Value Decomposition Method Year GLP Test substance	 = 236 - 247 °C at other: D1078/01 2003 no data
Test substance Reliability Flag 12.10.2006	 CAS No. 68938-07-8; Fatty acids, C9-13-neo- (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. Critical study for SIDS endpoint (9)
2.5 DENGITI	
Type Value Method Year GLP Test substance	= .92 g/cm ³ at 20 °C 2003 no data
Test substance Reliability	 CAS No. 68938-07-8; Fatty acids, C9-13-neo- (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.
⊢lag 12.10.2006	: Critical study for SIDS endpoint (9)
2.3.1 GRANULOMETRY	

2. Physico-Chemical Data

(6)

2.4 VAPOUR PRESSURE

Value Decomposition Method Year GLP Test substance	= .001061 hPa at 25 °C other (calculated) 2003
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 12.10.2006	Critical study for SIDS endpoint

2.5 PARTITION COEFFICIENT

Partition coefficient Log pow pH value Method Year GLP Test substance	 octanol-water = 3.3 - 5.2 at 25 °C other (calculated) 2003
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.	:	
рКа	:	4.8 at 25 °C
Description	:	
Stable	:	
Deg. product	:	

2. Physico-Chemical Data

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

2.7 FLASH POINT

Valu Typ Met Yea GLF Tes	ue e hod r s t substance	::	= 124 °C open cup other: COC ASTM D92 2003 no data	
Tes Reli	t substance ability	:	CAS No. 68938-07-8; Fatty acids, C9-13-neo- (2) valid with restrictions Although the original data were not retrieved and reviewed for quality, the were developed following acceptable test methods and therefore considered reliable.	еу
Flag 12.1) 0.2006	:	Critical study for SIDS endpoint	(9)
				(-)
2.8	AUTO FLAMMABIL	ITY		
2.9	FLAMMABILITY			
-				
2.10	EXPLOSIVE PROPE	ERT	IES	
2.11	OXIDIZING PROPER	RTIE	ES	
2.12	DISSOCIATION CO	NST	ANT	
Acie Met	d-base constant hod	:	4.8 other: calculated 8 / 31	

	Date 06.11.2006	
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	
	I he value was calculated based on the chemical structure as modeled be SPARC. This robust summary has a reliability rating of 2 because the d	by lat
	are calculated and not measured.	
12.10.2006		(1)
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, th were developed following acceptable test methods and therefore considered reliable 	ie

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

3.1.1 PHOTODEGRADATION

Type Light source Light spectrum Relative intensity INDIRECT PHOTOLYSIS Sensitizer Conc. of sensitizer Rate constant Degradation Deg. product Method Year GLP Test substance		Sun light nm based on intensity of sunlight OH 1500000 molecule/cm ³ = .0000000000103617 cm ³ /(molecule*sec) % after other (calculated) 2003
Method Result	:	other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04 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* OH- Rate Constant half-life (days) (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.
Test condition	:	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. Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.

3. Environmental Fate and Pathways

ld 68938-07-8 Date 06.11.2006

Test substance Reliability Flag 12.10.2006	 Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3 CAS No. 68938-07-8; Fatty acids, C9-13-neo- (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. Critical study for SIDS endpoint (6) 	
Type Light source Light spectrum Relative intensity Deg. product Method Year GLP Test substance	water nm based on intensity of sunlight other (calculated): Technical discussion	
Remark Result	 These data represent a key study for characterizing the potential of substances in the Neoacids C5 to C28 Category to undergo direct photodegradation. 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. 11 / 31	
3. Environmenta	I Fate and Pathways	ld 68938-07-8
--	---	---
		Date 06.11.2006
	Lyman, W. F. Reehl, and D. H. Rose Property Estimation Methods, McGra USA.	enblatt, eds., Handbook of Chemical aw-Hill Book Company, New York,
	Zepp, R. G. and D. M. Cline. 1977. R Aqueous Environment, Environ. Sci.	Rates of Direct Photolysis in the Technol., 11:359-366.
Test substance Flag 01.09.2006	 Boethling, R.S., Mackay, D. 2000. H Methods for Chemicals, CRC Press, Neoacids C5 to C28 Category memb Critical study for SIDS endpoint 	landbook of Property Estimation Boca Raton, FL, USA. pers (5)
3.1.2 STABILITY IN V	VATER	
Type t1/2 pH4 t1/2 pH7 t1/2 pH9 Deg. product Method	: abiotic : at °C : at °C : at °C : : : other: technical discussion	
Year GLP Test substance		
Remark Result	 These data represent a key study for substances in the Neoacids C5 to C2 Hydrolysis as a Function of Molecula 	r characterising the potential of 28 Category to undergo hydrolysis. ar Structure
	Hydrolysis of an organic molecule oc with water (H2O) to form a new carbo bond is cleaved (Gould, 1959; Harris is referred to as a nucleophilic substi group being replaced by the incomin- molecule.	ccurs when a molecule (R-X) reacts on-oxygen bond after the carbon-X s, 1982). Mechanistically, this reaction itution reaction, where X is the leaving g nucleophilic oxygen from the water
	Chemicals that are susecptible to hydrogen can be displaced by a nucleophilic surplice of the surplice of the surplice and the surplice of the surplice of the sulfonic acid esters and lactones, sulfonic acid esters (Neely, 1985). The renders a compound resistant to hydrogen surplice of the surplice of	drolysis contain functional groups that ubstitution reaction. Substances that alkyl halides, amides, carbamates, epoxides, phosphate esters, and he lack of a suitable leaving group Irolysis.
	Aliphatic acids are resistant to hydrol group that is hydrolytically reactive (H	lysis because they lack a functional Harris, 1982).
	References:	
	Gould, E.S. (1959), Mechanism and Reinhart and Winston, New York, NY	Structure in Organic Chemistry, Holt, /, USA.
	Harris, J.C. (1982), "Rate of Hydrolys Reehl, and D.H. Rosenblatt, eds., Ha Estimation Methods, McGraw-Hill Bo	sis," Chapter 7 in: W.J. Lyman, W.F. andbook of Chemical Property ook Company, New York, NY, USA.
Test substance Conclusion	 Neely, W. B. 1985. Hydrolysis. In: W. Environmental Exposure from Chemi Boca Raton, FL, USA. Neoacids C5 to C28 Category memb Hydrolysis will not contribute to the restriction of the restriction	. B. Neely and G. E. Blau, eds. icals. Vol I., pp. 157-173. CRC Press, pers emoval of neoacids from the

3. Environmental Fat	e and Pathways	ld Date	68938-07-8 06.11.2006
Flag : 01.09.2006	environment. Critical study for SIDS endpoint		
3.1.3 STABILITY IN SOIL			
3.2.1 MONITORING DATA			
3.2.2 FIELD STUDIES			
3.3.1 TRANSPORT BETWE	EN ENVIRONMENTAL COMPARTMENTS		
Type : Media : Air : Water : Soil : Biota : Soil : Method :	fugacity model level III other: air - sediment(s) - soil - water % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) other: Calculation according Mackay, Leve	4 111	
Method :	The EQC Level III model is a steady state determining how the medium of release aff III fugacity allows non-equilibrium condition media as steady state, and illustrate impor processes.	model that is fects environ ns to exist be tant transpor	useful for mental fate. Leve tween connected t and transformation
	Physicochemical input values for the mode EPIWIN Estimation v 3.04 program. Meas used where available and obtained from th data from the equilibrium model provide ba partitioning behavior of chemicals between compartments (i.e., air, water, soil, and sec	el were calcu ured input va le EPIWIN da asic informati la selected en diment).	lated using the alues were also atabase. Distribution on on the potentia vironmental
	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% discha	arge to wate	r.
Result :	Air - 0.26% Water - 41.5% Soil - 6.6% Sediment - 51.7%		
	10/01		

Reliability	 CAS No. 68938-07-8; Fatty acids, C9-13-neo- (2) valid with restrictions This robust summary has a reliability rating of 2 because the data are acculated and not measured
Flag	Critical study for SIDS endpoint
12.10.2006	(1)
Turne	
i ype Modia	: Tugacity model level 1 • 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 IÍ/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%
	AIF - 5.1% Water - 5.0%
	Sediment - 2.0%
	Suspended Sed - 0.06%
Testes!	Biota - <0.01%
Test substance Conclusion	 CAS No. 68938-07-8; Fatty acids, C9-13-neo- 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.
Reliability Flag	 (2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured. Critical study for SIDS endpoint

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 **BIODEGRADATION**

Type Inoculum Contact time Degradation Result Deg. product Method Year GLP Test substance	 aerobic activated sludge, domestic = 2.3 (±) % after 28 day(s) OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test" 1996 yes
Remark Result	 Test Type: Manometric Respirometry Test 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. % Degradation* Mean % Degradation Sample (day 28) (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 Reliability	 I est substance is considered not readily biodegradable. (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 Elimination Method Year GLP Test substance		= 3.16 other: calculated 2003
Method Test condition	:	Calculated values using BCFWIN version 2.13, a subroutine of the computer program EPIWIN version 3.04 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.
Test substance Reliability	:	Log Kow used = 4.89 CAS No. 68938-07-8; Fatty acids, C9-13-neo- (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 12.10.2006	:	Critical study for SIDS endpoint (6)

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type Species Exposure period Unit LC50 Limit test Analytical monitoring Method Year GLP Test substance		semistatic Oncorhynchus mykiss (Fish, fresh water) 96 hour(s) mg/l = 37.5 measured/nominal no yes OECD Guide-line 203 "Fish, Acute Toxicity Test" 2003 yes
Remark Result	:	Statistical Method: Bionomial Method 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.
Test condition	:	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 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<br 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.
Test substance Reliability Flag	:	Fish Mean Wt.= 0.460g. Mean Total length = 4.0cm, Test Loading = 0.535 g of fish/L. CAS No. 68938-07-8; Fatty acids, C9-13-neo- (1) valid without restriction Critical study for SIDS endpoint
12.10.2006		(1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4. Ecotoxicity

ld 68938-07-8 Date 06.11.2006

Type Species Exposure period Unit EC50 Limit Test Analytical monitoring Method Year GLP Test substance	 static Daphnia magna (Crustacea) 48 hour(s) mg/l = 62.2 measured/nominal no yes OECD Guide-line 202 2003 yes
Remark Result	 Statistical Method: Bionomial Method 48-hour EC50 = 62.2 mg/L (CI 45.6 - 84.9), based upon measured concentrations of mean of old and new samples.
Test condition	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 : 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.</th
Test substance Reliability Flag 12.10.2006	 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. CAS No. 68938-07-8; Fatty acids, C9-13-neo- (1) valid without restriction Critical study for SIDS endpoint

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"

4. Ecotoxicity	ld 68938-07-8 Date 06.11.2006
Year GLP Test substance	: 2003 : yes :
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 .
Result	 were determined using the ANOVA procedure of SAS. 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
	Mean CellNominalGrowth - 72 hrConc 72 hrConc. (mg/L)(% Inhibition)(cells/ml)Controln/a $1.2 \times 10E6$ 64.5 (62.4)* 3.9 $1.0 \times 10E6$ 125 (120) 4.9 $1.0 \times 10E6$ 247 (226) 27 $3.5 \times 10E5$ 531 (350) 51 $1.0 \times 10E5$ 1054 (432) 59 $6.5 \times 10E4$
Test condition	 *note - value in parentheses is mean measured concentration (mg/L) n/a - Not applicable 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

4. Ecoloxicity	ld 68938-07-8 Date 06.11.2006
	inoculated with \sim 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).
Test substance Reliability	 The pH ranged from 7.5 to 7.6 at test initiation and ranged from 6.6 to 7.0 at termination. CAS No. 68938-07-8; Fatty acids, C9-13-neo- (1) valid without restriction
Flag 12.10.2006	: Critical study for SIDS endpoint (3)
4.4 TOXICITY TO MICF	ROORGANISMS E.G. BACTERIA
4.5.1 CHRONIC TOXICIT	TY TO FISH
4.5.2 CHRONIC TOXICIT	Y TO AQUATIC INVERTEBRATES
4.6.1 TOXICITY TO SED	IMENT DWELLING ORGANISMS
4.6.2 TOXICITY TO TER	RESTRIAL PLANTS
4.6.3 TOXICITY TO SOIL	DWELLING ORGANISMS
4.0.4 TOX. TO OTHER R	ON MAMM. TERR. SPECIES
4.0.4 TOX. TO OTHER R	ON MAMM. TERR. SPECIES
4.7 BIOLOGICAL EFFE	ECTS MONITORING
4.7 BIOLOGICAL EFFE	ECTS MONITORING
4.7 BIOLOGICAL EFFI 4.8 BIOTRANSFORMA	ECTS MONITORING
4.7 BIOLOGICAL EFFI 4.8 BIOTRANSFORMA	ECTS MONITORING
 4.7 BIOLOGICAL EFFI 4.8 BIOTRANSFORMA 4.9 ADDITIONAL REM 	ECTS MONITORING
 4.7 BIOLOGICAL EFFI 4.8 BIOTRANSFORMA 4.9 ADDITIONAL REM 	ECTS MONITORING

5. Toxicity

Id 68938-07-8 Date 06.11.2006

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 Species Number of animals Vehicle Result Classification Method Year GLP Test substance		other: Magnusson-Kligman maximization test guinea pig not sensitizing 1993 no data
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

Туре	:	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
		21/31

5. Toxicity	ld 68938-07-8 Date 06.11.2006
Control group NOAEL	 other: Polyethylene glycol 200/distilled water (80%/20%) was administered to 10 animals at a level of 1 ml/kg body weight. = 300 - mg/kg bw OECD Guide line 407 "Repeated Dasa Oral Taxisity" Redent: 28 day or
Year GLP Test substance	 14-d Study" 1994 yes
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%)
Result	 Control: Polyethylene glycol 200/distilled water (80%/20%) was administered to 10 animals at a level of 1 ml/kg body weight. 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 doserelated 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 Conclusion	 CAS No. 68938-07-8; Fatty acids, C9-13-neo- Under condition of this study, fatty acids, C9-C13 neo does not cause significant toxic effects after repeated exposure
Reliability Flag 13.10.2006	 : (1) valid without restriction : Critical study for SIDS endpoint (12)

5.5 GENETIC TOXICITY 'IN VITRO'

:	Bacterial reverse mutation assay		
:	Ames Salmonella assay with and without metabolic activation and E.coli		
:	: 31.25 to 5000 ug/plate		
:			
:	with and without		
: negative			
:	OECD Guide-line 471		
:	1993		
:	ves		
:			
:	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.		
:	Species/strain tested: S. typhimurium TA 1535, 1537, 98, 100 and E. coli		
	WP2uvrA pKM101		
	Creation (call type) Det liver (CO) fraction		
	Species/cell type: Rat liver (59) fraction		
	Concentrations tested: 31.25 - 5000 μ g/plate + S9. All diluted in acetone		
	$\frac{1}{2} = \frac{1}{2} = \frac{1}$		
	Solubility of test substance was limited at concentrations of 2000 - 5000		
	ug/plate.		

5. Toxicity	ld 68938-07-8
	Date 06.11.2006
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 ware developed following acceptable test methods and therefore
	considered reliable.
Flag 19.10.2006	: Critical study for SIDS endpoint (13)
Туре	: Chromosomal aberration test
System of testing	: Chinese Hamster Ovary (CHO) cells
Test concentration	
Metabolic activation	: with and without
Result	:
Method	:
Year	: 1994
Test substance	: yes
Result	: In the absence of rat liver S9, mitotic inhibition was 62% at 218.75 μ g/ml and in a second experiment 62% at 250 μ g/ml. In the presence of S9, no
	mitotic inhibition at 1000 μ g/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
Test substance Conclusion	 Dose selection was based on a preliminary study covering doses of 3.42 to 1750 µg/ml (solubility limit in the medium). CAS No. 68938-07-8; Fatty acids, C9-13-neo- Fatty acids, C9-C13 neo induces chromosomal aberrations in CHO cells in the presence of S9; however, no chromosomal aberration was observed in
Reliability	 the absence of S9. (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

5. Toxicity

19.10.2006

5.6 GENETIC TOXICITY 'IN VIVO'

Type Species Sex Strain Route of admin. Exposure period Doses Result Method Year GLP Test substance	 other: Micronucleus test in vivo mouse male/female other: Swiss (Charles River CD-1) other: oral gavage 0, 2000 mg/kg (limit dose); diluted in PEG 200/water (80/20 w/w) negative 1995 yes 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 all 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 Conclusion	 CAS No. 68938-07-8; Fatty acids, C9-13-neo- 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 19.10.2006	: Critical study for SIDS endpoint (16)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Туре	:	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

(15)

24 / 31

5. Toxicity	ld 68938-07-8 Date 06.11.2006
Duration of test Doses Control group Method Year GLP Test substance	 One generation 0, 600, 1200, 2500, 5000 ppm in diet yes 1998 yes
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
Result	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.
Test condition	 Maternal and Offspring NOAEL = 1200 ppm 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 Conclusion	 Analog material: CAS No. 3302-10-1; Isononanoic acid 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 Flag 13.10.2006	 (1) valid without restriction Critical study for SIDS endpoint (8)

5. Toxicity

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses	
---	--

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

9. Referenc	Id 68938-07-8 Date 06.11.2006
(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



Ĺ

2006 NOV 14 AM 10: 55

IUCLID

Data Set

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

1. General Information

ld 72480-45-6 Date 06.11.2006

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

erre	эе	text
2	ee tre	e tree

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 Molecular weight Petrol class	: : : :	C19H38O2 298.51
Flag 13.10.2006	:	Critical study for SIDS endpoint

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid

	Date 06.11.2006
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
13.10.2006	
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 rang of C9 through C28 and boiling in the range of approximately 225 to 387°
13.10.2006	
Purity type	• typical for marketed substance
CAS-No	: 72480-45-6
EC-No	• • • • • • • • • • • • • • • • • • •
EINECS-Name	: Fatty acids, C9-28-neo-
wolecular formula Value	
Function of additive	:
Remark 13.10.2006	: No additives present
1.5 TOTAL QUANTIT	Y
1.6.1 LABELLING	

1. General Informat	tion	ld Date	72480-45-6 06.11.2006		
1.6.2 CLASSIFICATION					
1.6.3 PACKAGING					
1.7 USE PATTERN					
Type of use Category	: industrial : Chemical industry: used in synthes	sis			
Remark 13.10.2006	: Primary use for fatty acids, C9-28, industry.	neo- is in the paint a	nd coatings		
1.7.1 DETAILED USE PA	TTERN				
1.7.2 METHODS OF MAN	IUFACTURE				
1.8 REGULATORY ME	1.8 REGULATORY MEASURES				
1.8.1 OCCUPATIONAL E	XPOSURE LIMIT VALUES				
1.8.2 ACCEPTABLE RES	IDUES LEVELS				
1.8.3 WATER POLLUTIO	Ν				
1.8.4 MAJOR ACCIDENT	HAZARDS				
1.8.5 AIR POLLUTION					
1.8.6 LISTINGS E.G. CHE					
1.9.1 DEGRADATION/TR	ANSFORMATION PRODUCTS				
1.9.2 COMPONENTS					
1.10 SOURCE OF EXPO	SURE				

1. General Information Id 72480-45-6 Date 06.11.2006 1.11 ADDITIONAL REMARKS 1.12 LAST LITERATURE SEARCH 1.13 REVIEWS

2.1 MELTING POINT

Value Sublimation Method Year GLP Test substance	 = 37 - 76 °C other: ASTM D97 2003 no data
Test substance Reliability	 CAS No. 72480-45-6; Fatty acids, C9-28-neo- (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 16.10.2006	: Critical study for SIDS endpoint (4)
2.2 BOILING POINT	
Value Decomposition Method Year GLP Test substance	 = 236 - 247 °C at other: D1078/01 2003 no data
Test substance Reliability Flag 16.10.2006	 CAS No. 72480-45-6; Fatty acids, C9-28-neo- (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. Critical study for SIDS endpoint (4)
Type Value Method Year GLP Test substance	 density = .92 g/cm³ at 20 °C 2003 no data
Test substance Reliability	 CAS No. 72480-45-6; Fatty acids, C9-28-neo- (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. Critical study for SIDS endpoint
гау 16.10.2006	. Childai suudy loi SIDS enupoint (4)
2.3.1 GRANULOMETRY	

2. Physico-Chemical Data

ld 72480-45-6 Date 06.11.2006

(3)

2.4 VAPOUR PRESSURE

Value Decomposition Method Year GLP Test substance		= .00000000023061 hPa at 25 °C other (calculated) 2003
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 16.10.2006	:	Critical study for SIDS endpoint

2.5 PARTITION COEFFICIENT

Partition coefficient Log pow pH value Method Year GLP Test substance	 octanol-water = 3.3 - 6 at 25 °C other (calculated) 2003
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.	:	
рКа	:	4.9 at 25 °C
Description	:	
Stable	:	
Deg. product	:	

2. Physico-Chemical Data

	Method Year GLP Test substance	: :	other: calculated 2003		
	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 Reliability	:	CAS No. 72480-45-6; Fatty acids, C9-28-neo- (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 16.10.2006	:	Critical study for SIDS endpoint	(3)	
2	2.6.2 SURFACE TENSIO	N			
2	2.7 FLASH POINT				

Valu Typ Met Yea GLF Tes	ue he hod r s t substance		= 118.3 °C closed cup other: PMCC ASTM D93 2003 no data	
Tes Reli	t substance iability	:	CAS No. 72480-45-6; Fatty acids, C9-28-neo- (2) valid with restrictions Although the original data were not retrieved and reviewed for quality, the were developed following acceptable test methods and therefore considered reliable.	у
Flaç 16.1	g 10.2006	:	Critical study for SIDS endpoint ((4)
2.8	AUTO FLAMMABIL	ITY		
2.9	FLAMMABILITY			
2.10	EXPLOSIVE PROPE	ERT	IES	
2.11	OXIDIZING PROPER	RTIE	ES	
2.12	DISSOCIATION CO	NST	TANT	
Acio Met	d-base constant hod	:	4.9 other: calculated 8 / 23	

Year	: 2003
GLP Test substance	
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 dat
40.40.0000	are calculated and not measured.
16.10.2006	(

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type Light source Light spectrum Relative intensity INDIRECT PHOTOLYSIS Sensitizer Conc. of sensitizer Rate constant Degradation Deg. product Method Year GLP Test substance		Sun light nm based on intensity of sunlight OH 1500000 molecule/cm ³ = .00000000000202531 cm ³ /(molecule*sec) % after other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04 2003
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* OH- Rate Constant half-life (days) (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.
Test condition	:	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. Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.
		Temperature: 25°C
		10 / 23

ld 72480-45-6 Date 06.11.2006

Test substance Reliability Flag 16.10.2006	 Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3 CAS No. 72480-45-6; Fatty acids, C9-28-neo- (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. Critical study for SIDS endpoint (3)
Type Light source Light spectrum Relative intensity Deg. product Method Year GLP Test substance	water nm based on intensity of sunlight other (calculated): Technical discussion
Remark	 These data represent a key study for characterizing the potential of substances in the Neoacids C5 to C28 Category to undergo direct photodegradation. Photolysis as a Function of Molecular Structure
	 Protocysis as a function of Notecular 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. However, the assorption 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 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.
	Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

3. Environmental I	Fate and Pathways	ld 72480-45-6 Date 06.11.2006
	Property Estimation Methods, McGraw-I USA.	Hill Book Company, New York,
	Zepp, R. G. and D. M. Cline. 1977. Rate Aqueous Environment, Environ. Sci. Teo	es of Direct Photolysis in the chnol., 11:359-366.
Test substance Flag 01.09.2006	 Boethling, R.S., Mackay, D. 2000. Hand Methods for Chemicals, CRC Press, Boo Neoacids C5 to C28 Category members Critical study for SIDS endpoint 	dbook of Property Estimation ca Raton, FL, USA.
3.1.2 STABILITY IN WA	TER	
Type t1/2 pH4 t1/2 pH7 t1/2 pH9 Deg. product Method Year GLP Test substance	abiotic at °C at °C at °C other: technical discussion	
Remark Result	 These data represent a key study for chasubstances in the Neoacids C5 to C28 C Hydrolysis as a Function of Molecular Statement 	aracterising the potential of Category to undergo hydrolysis. tructure
	Hydrolysis of an organic molecule occur with water (H2O) to form a new carbon-o bond is cleaved (Gould, 1959; Harris, 19 is referred to as a nucleophilic substitution group being replaced by the incoming no molecule.	rs when a molecule (R-X) reacts oxygen bond after the carbon-X 982). Mechanistically, this reaction on reaction, where X is the leaving ucleophilic oxygen from the water
	Chemicals that are susecptible to hydrol can be displaced by a nucleophilic subst have a potential to hydrolyze include alk carboxylic acid esters and lactones, epo sulfonic acid esters (Neely, 1985). The la renders a compound resistant to hydroly	lysis contain functional groups that titution reaction. Substances that yl halides, amides, carbamates, oxides, phosphate esters, and ack of a suitable leaving group ysis.
	Aliphatic acids are resistant to hydrolysis group that is hydrolytically reactive (Hari	s because they lack a functional ris, 1982).
	References:	
	Gould, E.S. (1959), Mechanism and Stru Reinhart and Winston, New York, NY, U	ucture in Organic Chemistry, Holt, ISA.
	Harris, J.C. (1982), "Rate of Hydrolysis,' Reehl, and D.H. Rosenblatt, eds., Hand Estimation Methods, McGraw-Hill Book	" Chapter 7 in: W.J. Lyman, W.F. book of Chemical Property Company, New York, NY, USA.
Test substance Conclusion	 Neely, W. B. 1985. Hydrolysis. In: W. B. Environmental Exposure from Chemical Boca Raton, FL, USA. Neoacids C5 to C28 Category members Hydrolysis will not contribute to the remore environment. 	Neely and G. E. Blau, eds. s. Vol I., pp. 157-173. CRC Press, s oval of neoacids from the

3. Environmental Fa	te and Pathways	ld Date	72480-45-6 06.11.2006
Flag 01.09.2006	: Critical study for SIDS endpoint		(1)
3.1.3 STABILITY IN SOIL			
3.2.1 MONITORING DATA			
3.2.2 FIELD STUDIES			
3.3.1 TRANSPORT BETW	EEN ENVIRONMENTAL COMPARTMENT	S	
Type Media Air Water Soil Biota Soil Method Year Method	 fugacity model level III other: air - sediment(s) - soil - water % (Fugacity Model Level I) % (Fugacity Model Level II/III) other: Calculation according Mackay, Level 2003 The EQC Level III model is a steady state determining how the medium of release III fugacity allows non-equilibrium condit media as steady state, and illustrate im processes. Physicochemical input values for the m EPIWIN Estimation v 3.04 program. Me used where available and obtained from data from the equilibrium model provide partitioning behavior of chemicals betwee compartments (i.e., air, water, soil, and 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 - 720000 hrs 	evel III ate model that is affects environ itions to exist be portant transpor odel were calcul easured input va n the EPIWIN da basic informati een selected en sediment).	s useful for mental fate. Level tween connected t and transformation lated using the alues were also atabase. Distribution on on the potential vironmental
Result	: Air - 0.01% Water - 20.3%		
Test substance	Soil - 10.2% Sediment - 69.5% : CAS No. 72480-45-6; Fatty acids, C9-2	8-neo-	
	13 / 23		

Reliability Flag	 (2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured. Critical study for SIDS endpoint
16.10.2006	(6)
Type Media Air Water Soil Biota Soil Method Year	 fugacity model level I other: air - biota - sediment(s) - soil - water % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level I) % (Fugacity Model Level II/III) % (Fugacity Model Level II/III) other: Calculation according Mackay, Level I 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 Conclusion	 CAS No. 72480-45-6; Fatty acids, C9-28-neo- 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.
Reliability	 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. (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
10.10.2006	(6)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 **BIODEGRADATION**

Type Inoculum	:	aerobic
Remark	:	No data are available

16.10.2006

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF Elimination Method Year GLP Test substance	: = 3.16 - : : other: calculated : 2003
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.
Tast substance	Log Kow used = 4.7
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. Ecotoxicity

ld 72480-45-6 Date 06.11.2006

- 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. То	xicity	ld Date	72480-45-6 06.11.2006
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. Toxicity

ld 72480-45-6 Date 06.11.2006

5.11 ADDITIONAL REMARKS

6. Analyt. Meth. for Detection and Identified	cation
---	--------

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against	Target Org. and Intended Uses	5
-----------------	-------------------------------	---

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

9. References

- (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