

201-14018C

I U C L I D

Data Set

05 AUG 31 PM 2:23

00000000

Existing Chemical : ID: 90438-79-2
CAS No. : 90438-79-2
TSCA Name : Acetic acid, C6-8-branched alkyl esters
Molecular Formula : Unspecified

Producer related part
Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 07.12.2000

Substance related part
Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 07.12.2000

Status :
Memo : ExxonMobil HPV

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Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the alkyl acetates category.

Remark : Alkyl Acetates follow a regular pattern as a result of synthesis and structural similarity. Aliphatic, monohydric alcohols are reacted with acetic acid to form the corresponding acetate esters (CH₃COOR).
Members associated with this template category are:
88230-35-7 Hexanol, acetate, branched and linear
90438-79-2 Acetic acid, C6-8 branched alkyl esters
108419-32-5 Acetic acid, C7-9 branched alkyl esters
108419-33-6 Acetic acid, C8-10 branched alkyl esters
108419-34-7 Acetic acid, C9-11 branched alkyl esters
108419-35-8 Acetic acid, C11-14 branched alkyl esters

07.12.2000

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

C6 - C8 branched alkyl acetate ester

27.02.2004

Exxate 700

27.02.2004

oxo-heptyl acetate

04.06.2004

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

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. General Information

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1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

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Date 19.04.2005

2.1 MELTING POINT

Value : = -50 °C
Sublimation :
Method : other: Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no data
Test substance : other TS: C7 methyl-branched alkyl acetate ester

Method : Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle.

Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

The Gold and Ogle Method simply uses the formula
 $T_m = 0.5839T_b$, where T_m is the melting point in Kelvin and T_b is the boiling point in Kelvin.

Remark : EPIWIN is used and advocated by the USEPA for chemical property estimation.

Test substance : C7 methyl-branched alkyl acetate ester
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
19.04.2005 (3)

2.2 BOILING POINT

Value : = 176 - 200 °C at 1013 hPa
Decomposition :
Method : other: ASTM D1078 Mod
Year :
GLP : no data
Test substance : other TS

Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Reliability : (4) not assignable
This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.

Flag : Critical study for SIDS endpoint
04.06.2004 (15)

2.3 DENSITY

Type : relative density
Value : = .87 at 20 °C
Method : other: ASTM D891
Year :
GLP : no data

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Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Reliability : (4) not assignable
This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.

Flag : Critical study for SIDS endpoint
19.04.2005 (15)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = 1.035 hPa at 25 °C

Decomposition :

Method : OECD Guide-line 104 "Vapour Pressure Curve"

Year : 1995

GLP : yes

Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Result : Sorbent trap extraction samples were analyzed using gas chromatography.

Average Vapor Pressure per temperature:

24 Deg C (room temp) 96.38 Pa

35 Deg C 214.3 Pa

45 Deg C 438.8 Pa

Test condition : 25 Deg C 103.5 Pa (estimated from linear regression)
The test substance was coated onto glass beads, which were then transferred to saturator columns. Three columns were prepared for each temperature evaluation (9 total). The Vapor Pressure was evaluated at temperatures of 24, 35, and 45 Deg C. A stream of inert carrier gas (N2) was passed over the separator columns and became saturated with the test substance vapors. The test substance vapors were then adsorbed to charcoal sorbent tubes.
Sorbent tubes were extracted with 2% acetone in carbon disulfide.

Vapor pressure determination interval was 2 hours at 24 Deg C and 1 hour at 35 and 45 Deg C. The N2 flow rate was 50ml/min at each temperature evaluation.

Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint
19.04.2005 (8)

Value : = .68 hPa at 25 °C

Decomposition :

Method : other (calculated): Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04

Year :

GLP : no data

Test substance : other TS

Test condition : Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods

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use boiling point for the calculation.

The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990.

A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.

Test substance : CAS No. 90438-79-2; Acetic acid, C6-8 branched and linear
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
04.06.2004 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : 3.9 - 4.2 at °C
pH value :
Method : OECD Guide-line 117 "Partition Coefficient (n-octanol/water), HPLC Method"
Year : 1989
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Result : The test substance eluted as several groups. One group was estimated to have a Log Pow of < 0.3. The second group had a Log Pow values ranging from 1.7 to 4.4. The three major components C6, C7, C8 acetates had Log Pow values of 3.9, 4.0, and 4.2 respectively.
The retention time for the 3 major components were 7.66, 8.04, and 8.71 minutes.
All values were measured using High Performance Liquid Chromatography (HPLC).
Test condition : The test substance was evaluated as a 5.3% solution in HPLC grade methanol. Six reference compounds were also evaluated in a combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) of 75% methanol and 25% distilled water. The pH of both solutions was 6.5.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005 (6)

Partition coefficient : octanol-water
Log pow : = 3.32 at 25 °C
pH value :
Method : other (calculated): Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year :
GLP : no data
Test substance : other TS
Test condition : Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is 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-

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92.
Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
04.06.2004 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 158 mg/l at 20 °C
pH value : 3.5 - 4.9
concentration : at 20 °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : OECD Guide-line 105
Year : 1995
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Result : Water solubility = 158 mg/L. Samples measured over three equilibration days on three separate replicates.
Day 1 154 mg/L pH 3.5
Day 2 154 mg/L pH 4.9
Day 3 162 mg/L pH 4.3

Test condition : The clear aqueous solution was analytically measured by gas chromatography using mass selective detection (GC-MSD).
: A total of 9 test systems were prepared. Three replicates for each of three equilibration days. The test systems consisted of glass distilled water and a loading of ~600mg/L of test substance. The test vessels were 25ml screw cap centrifuge tubes containing ~30ml of solution (no headspace). The test systems were agitated on an incubator shaker for the designated number of days at 30 Deg C, between 25 and 50 rpm. Samples were then transferred to a 20 Deg C incubator and agitated an additional 24 hours. The solutions were then centrifuged at 5000 rpm for 15 minutes and returned to the 20 Deg C incubator for another hour to ensure correct temperature at sampling. The surface test material and the next 10-15 ml were removed. The analytical samples were removed from the remaining (bottom) solution into a headspace sample vial.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005 (7)

Solubility in : Water
Value : = 102 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :

2. Physico-Chemical Data

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Deg. product :
Method : other: Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year :
GLP : no data
Test substance : other TS
Test condition : Water Solubility is calculated by the WSKOWWIN subroutine, which is 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. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

04.06.2004

(3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type : water
Light source : Sun light
Light spectrum : nm
Relative intensity : based on intensity of sunlight
Deg. product :
Method : other (calculated): Technical Discussion
Year :
GLP : no
Test substance : other TS: C7 methyl-branched alkyl acetate ester

Remark : These data represent a key study for characterising the potential of substances in the Alkyl Acetates C6 to C13 category to undergo direct photodegradation.

Result : Photolysis as a Function of Molecular Structure

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

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

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

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

Substances in the Alkyl Acetate C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb only in the far UV region, below 220 nm, (Boethling and Mackay, 2000) and therefore will not undergo direct photolysis. These data indicate that photolysis will not significantly contribute to the degradation of alkyl acetate esters in the aquatic environment.

References

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

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York,

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USA.

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

Test substance : CAS No. 90438-79-2; Acetic acid, C6-8 branched and linear
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Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .000000000088486 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no
Test substance : other TS: C7 methyl-branched alkyl acetate ester

Result : Atmospheric Oxidation Potential

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

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

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

Calculated* half-life (hrs)	OH- Rate Constant (cm ³ /molecule-sec)
14.5	8.85 E-12

References:

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

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

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

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on

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the structure-activity relationship methods developed by R. Atkinson.

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

Test substance : C7 methyl-branched alkyl acetate ester
Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.

Flag : Critical study for SIDS endpoint
19.04.2005 (3)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at 50 °C
t1/2 pH7 : = 24.3 day(s) at 50 °C
t1/2 pH9 : = 5.3 day(s) at 30 °C
t1/2 pH 9 : = 15.6 - 16 day(s) at 20 °C
Deg. product : not measured
Method : OECD Guide-line 111 "Hydrolysis as a Function of pH"
Year : 1997
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Result : Hydrolysis at pH 4 is stable (<10% degradation over 5 days).

Test condition : Test substance hydrolysis was observed at pH 9 and a slower but measurable hydrolysis occurred at pH 7.
The hydrolysis of the test substance was evaluated at 3 relevant pH values. A preliminary test at pH values of 4, 7 and 9, showed stability at pH 4. A definitive test was performed at pH values of 7 and 9 at varying temperatures (20 and 30 Deg C for pH 9; 40 and 50 Deg C for pH 7). Sufficient volumes of test substances stock solution were added to buffer solution to yield nominal concentration less than 60ug/L (40-53 ug/L) (half of expected water sol. conc.). Samples were stored in the dark in laboratory incubators and the temperature recorded daily.

Test substance : Test vessels were sterilized VOA vials containing buffer solutions of the test substance, with no headspace.
CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Conclusion : Hydrolysis of the test substance is not expected to be a significant mechanism of abiotic degradation in natural bodies of water where the temperature is generally less than 20 Deg C and the pH is at or below 7.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
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3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 1998

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 = 158.24 g/mol
 Water solubility = 102 mg/L
 Vapour pressure = 68 Pa
 log Kow = 3.32
 Melting point = -50 deg C

Result : Air- 88.0%
 Water- 4.1%
 Soil- 7.7%
 Sediment - 0.2%
 Suspended Sed - <0.01%
 Biota - <0.01%

Test substance : C7 methyl-branched alkyl acetate ester
Reliability : (2) valid with restrictions
 This robust summary has a reliability rating of 2 because the data are calculated and not measured.

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3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type :
Inoculum : activated sludge, domestic
Contact time : 28 day(s)
Degradation : (±) % after
Result :
Deg. product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year : 1993

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- GLP** : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Result** : Test material was readily biodegradable. Half-life was <1 week. By day 28, 77% degradation of the test material was observed. 10% biodegradation was achieved on day 1, 50% biodegradation on approximately day 5. 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.

	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	73.5, 80.4, 77.4	77.1
Na Benzoate	76.0, 78.3	77.1

- * replicate data
- Source** : ExxonMobil Chemicals
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 52mg/L. Sodium benzoate (positive control) concentration was 52mg/L.
Test temperature was 22 +/- 1 Deg C.
All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
- Reliability** : (1) valid without restriction
Flag : Critical study for SIDS endpoint
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3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

- Species** : other: see remark
Exposure period : at °C
Concentration :
BCF : = 63
Elimination :
Method : other: calculation
Year :
GLP : no data
Test substance : other TS: C7 methyl-branched alkyl acetate ester
- Remark** : A log BCF of 1.8 (BCF = 63) is calculated. C7 methyl-branched alkyl acetate ester in the aquatic environment is expected to have a low potential for bioaccumulation. The SMILES notation used was
CC(=O)OCCCC(C)CC
- Reliability** : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are

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Flag
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calculated and not measured.
: Critical study for SIDS endpoint

(2)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : semistatic
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 8.18 measured/nominal
Limit test :
Analytical monitoring : yes
Method : OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year : 1992
GLP : yes
Test substance : other TS: CAS No. 90438-79-2, C6 - C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Result : 96 hour LC50 = 8.18mg/L (95% CI 5.85 to 11.4) based upon measured values.

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

The fish were slightly smaller than the guideline suggestion of 4.0 to 6.0cm, which were purposely selected to help maintain oxygen levels in the closed system.

Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
1.2	0
1.49	0
5.39	2
21.1	10
43.6	10

*10 fish added at test initiation

Statistical Method: Trimmed Spearman Karber Method

Test condition : Individual test concentrations were prepared by adding the test substance, weighed on teflon disks, to 12 L of laboratory blend water in 13L glass aspirator bottles. The solutions were mixed for 24 hours at room temp (20-24 Deg C) with a vortex of <10% (3 cm vortex). Mixing was performed using a magnetic stir plate and teflon stir bar. After mixing, the solutions were allowed to settle for one hour and the Water Accommodated Fraction (WAF) was removed via port at the bottom of vessel. Test vessels were 4.0L aspirator bottles containing 4.0L of solution (no headspace). Test vessels were sealed with foil covered stoppers. Two replicates of each concentration were tested, each containing 5 fish. Approximately 80% of each solution was renewed daily from a freshly prepared WAF. Nominal treatment levels were control, 2.0, 4.5, 10.0, 23.0, and 50.0mg/L, which measured: 1.2, 1.49, 5.39, 21.1, and 43.6mg/L, respectively, and are based on the mean of samples taken from the new and old solutions. Test temperature was 13.6 Deg C. Lighting was 16 hrs light and 8 hrs dark. Dissolved oxygen was 8.3 to 10.4mg/L for "new" solutions and 4.5 to 7.9mg/L for "old" solutions. The pH ranged from 7.3 to 8.4 for "new" solutions and 6.7 to 7.6 for "old" solutions.

Fish supplied by Thomas Fish Co.; age = approximately 6 weeks; mean wt.=0.319g; mean total length=3.5cm; test loading=0.399g of fish/L.

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

19.04.2005

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4. Ecotoxicity

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4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

- Type** : other: Activated sludge - Respiration Inhibition
Species : activated sludge of a predominantly domestic sewage
Exposure period : 30 minute(s)
Unit : mg/l
Analytical monitoring : yes
Method : OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year : 1997
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Result** : No appreciable inhibition of respiration was measured. The controls were within 11.24% of their mean oxygen consumption rate and the EC50 for the reference substance was 20.8mg/L. Both values fall within the acceptable ranges for study validity (Controls within 15%, and positive substance between 5-30mg/L)
- Test condition** : The test solution consisted of synthetic sewage, activated sludge and reverse osmosis water. To this mixture, the appropriate amount of reference stock or test substance was added (except controls). The test treatments were aerated throughout the 30-minute exposure. After the 30 minute contact time, the contents were poured into a BOD bottle and the Dissolved Oxygen (DO) concentration was measured for 10 minutes or until a DO level of 2.5mg/L was achieved. The respiration rate was determined by the linear slope of DO level vs time.
- The positive control (3,5-DCP) was tested at concentrations of 5, 15 and 30 mg/L. The test substance was evaluated at concentrations of 5, 10, 25, and 50 mg/L.
- Test substance** : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Conclusion** : The test substance did not inhibit the respiration of the sludge medium.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005 (10)
- Type** : soil
Species : aerobic microorganisms
Exposure period : 28 day(s)
Unit :
Analytical monitoring : yes
Method : OECD Guide-line 216
Year : 2001
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Result** : Following an initial rise in ammonium concentrations in the soil of all groups, nitrogen transformation was evident from the subsequent decline in ammonium concentrations and gradual increase in nitrate concentrations over the study period.

Test condition

Statistical evaluation of the ammonium and nitrate data found a number of statistically significant differences in treated soil groups when compared with the non-treated control soil. However, at the end of the 28 day study period, the deviation in measured activity in soils treated with the test substance at 1x PEC (Group 2) and 5x PEC (Group 3) compared to non-treated control soil (Group 1) was less than 25% for both ammonium (0% for Group 2 and Group 3) and for nitrate (-1.12% and -6.41% for Group 2 and Group 3 respectively).

At the end of the 28 day study period, test soil "treated" with acetone as a solvent control showed values that were comparable (less than 25% different) to the non-treated control soil (Group 1) indicating that the use of acetone as a solvent had not adversely affected the test soil in this study.

: The test substance (TS) was tested at two treatment concentrations, the lower treatment concentration was equal to the maximum Predicted Environmental Concentration (PEC = 600 ml TS/hectare) and the higher treatment concentration was equal to 5x PEC (3 litres TS/hectare). The test soil was a sandy loam soil obtained from a site at Manningtree, Essex, England which had received no pesticides or fertilisers for at least 3 years prior to sampling.

To determine nitrogen transformation, non-treated control soil (Group 1) and soils treated with the test substance (Group 2 = 1x PEC, Group 3 = 5x PEC), were incubated in the dark at $20 \pm 2^\circ\text{C}$ as bulk samples. Each soil group was amended with lucerne meal, as a nitrogen source, at the time of preparation:

Group 1 - 2kg soil + lucerne meal + water

Group 2 - 2kg soil + lucerne meal + water containing 1x PEC

Group 3 - 2kg soil + lucerne meal + water containing 5x PEC

To achieve satisfactory incorporation of the test substance into the test soil, the test substance was first mixed with acetone and then transferred into the distilled water addition (60.7 g distilled water) required to amend the moisture content of the test soil to 40% of its maximum water holding capacity and this water was then sprinkled onto the soil and mixed in thoroughly.

Triplicate portions of each soil group were sampled within 6 hours (Day 0), 7, 14 and 28 days after preparation and then extracted for analysis of ammonium, nitrite and nitrate concentrations using a continuous flow colorimetric autoanalyser.

Analysis of soil

Sand (63 mm - 2 mm): 74.13%

Silt (2 mm - 63 mm): 20.36%

Clay (<2 mm): 5.51%

pH: 6.4

Organic carbon: 0.6%

Maximum water holding capacity: 26.1%

Cation exchange capacity (mEq/100 g): 7.4

Analysis of soil microbial biomass:

Total biomass (BC) mg C/kg soil: 115.17

Microbial biomass: 1.92%

(Total soil organic carbon = 0.6 %)

Test substance

: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

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- Conclusion** : Based on the results of this study, under anticipated conditions of field use equivalent to both 1x the PEC and 5x the PEC, the test substance did not exhibit a long-term influence on nitrogen transformation activity in soil.
- Reliability Flag** : (1) valid without restriction
19.04.2005 : Critical study for SIDS endpoint (16)
- Type** : soil
Species : aerobic microorganisms
Exposure period : 28 day(s)
Unit :
Analytical monitoring Method : yes
: OECD Guide-line 217
Year : 2001
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Result** : Statistical evaluation of the carbon transformation data found no statistically significant differences between the test soil treated with the test substance at 1x PEC when compared with the non-treated control soil. Statistical evaluation showed statistically significant increased levels of carbon transformation for the 5x PEC treated soil when compared with the non-treated control soil on Days 7, 14 and 28.
- At the end of the 28 day study period, the deviations in carbon transformation in soils treated with the test substance at 1x PEC (Group 2) compared to non-treated control soil (Group 1) were less than 25%, ranging from -5.5% to +3.4%. However carbon transformation in soil treated with the test substance at 5x PEC (Group 3) was substantially increased on Day 28 compared to non-treated control soil (Group 1), ranging from +27.0% to +109.2%.
- At the end of the 28 day study period, test soil "treated" with acetone as a solvent control showed values that were comparable (less than 25% different) to the non-treated control soil (Group 1) indicating that the use of acetone as a solvent had not adversely affected the test soil in this study.
- Test condition** : The test substance (TS) was tested at two treatment concentrations, the lower treatment concentration was equal to the maximum Predicted Environmental Concentration (PEC = 600 ml TS/hectare) and the higher treatment concentration was equal to 5x PEC (3 litres TS/hectare). The test soil was a sandy loam soil obtained from a site at Manningtree, Essex, England which had received no pesticides or fertilisers for at least 3 years prior to sampling.
- To determine carbon transformation, non-treated control soil (Group 1) and soils treated with the test substance (Group 2 = 1x PEC, Group 3 = 5x PEC), were incubated in the dark at $20 \pm 2^\circ\text{C}$ as bulk samples:
- Group 1 - 2kg soil + lucerne meal + water
Group 2 - 2kg soil + lucerne meal + water containing 1x PEC
Group 3 - 2kg soil + lucerne meal + water containing 5x PEC
- To achieve satisfactory incorporation of the test substance into the test soil, the test substance was first mixed with acetone and then transferred into the distilled water addition (60.7 g distilled water) required to amend the moisture content of the test soil to 40% of its maximum water holding capacity and this water was then sprinkled onto the soil and mixed in thoroughly.
- Triplicate portions of each soil group were sampled on Day 0, 7, 14 and 28 and treated with glucose to elicit an immediate glucose induced maximum

respiratory response. Respiration rates were determined at regular intervals over 12 consecutive hours using an ADC 2250 Infrared Gas Analyser.

Analysis of soil

Sand (63 mm - 2 mm): 74.13%
 Silt (2 mm - 63 mm): 20.36%
 Clay (<2 mm): 5.51%
 pH: 6.4
 Organic carbon: 0.6%
 Maximum water holding capacity: 26.1%
 Cation exchange capacity (mEq/100 g): 7.4

Analysis of soil microbial biomass:

Total biomass (BC) mg C/kg soil: 115.17
 Microbial biomass: 1.92%
 (Total soil organic carbon = 0.6 %)

- Test substance** : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Conclusion** : Based on the results of this study, under anticipated conditions of field use equivalent to 1x PEC, the test substance did not exhibit a long-term influence on carbon transformation activity in soil. When applied at a rate equivalent to 5x PEC, the test substance did show a stimulation of carbon transformation activity by soil microorganisms. This increase in carbon transformation activity as measured by an increase in carbon dioxide evolution is believed to have resulted from the mineralization of test substance by the soil microbial population.
- Reliability Flag** : (1) valid without restriction
 19.04.2005 : Critical study for SIDS endpoint (16)

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

- Species** : other terrestrial plant: Glycine max (soybean)
Endpoint : other: emergence / growth
Exposure period : 17 day(s)
Unit : mg/kg soil dw
LL50 : > 1562 measured/nominal
EL50 : > 1562 measured/nominal
Method : OECD Guide-line 208 "Terrestrial Plants, Growth Test"
Year : 2001
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Method** : The statistical method used to calculate the LL50 values was a maximum

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Result

likelihood analysis based on Finney, D.J., 1971. Probit Analysis, 3rd Edition, London: Cambridge University Press. The EL50 values were determined using the linear interpolation method (Norberg-King, T.J., A Linear Interpolation Method for Sublethal Toxicity: The Inhibition Concentration (ICp) Approach (Version 2.0). July 1993. U.S. Environmental Protection Agency, Environmental Research Laboratory, Duluth MN).

- : The LL50 (Lethal Loading 50) for Soybean (Glycine max) > 1562 mg/Kg.
- The EL50 (Effect Loading 50) for Soybean (Glycine max) > 1562 mg/Kg.

The soybean did not exhibit a lethal effect by test termination at the highest loading tested (1562 mg/Kg). The test substance did exhibit an effect on growth compared to the control (30 percent reduction), but not sufficient to cause a 50 percent effect.

Test condition

The LL50 (Lethal Loading 50) is the test substance loading level, which exhibits 50% emergence of the test species as compared to the control for a specific exposure period. The EL50 (Effect Loading 50) is the test substance loading level, which exhibits 50% growth of the test species based on weight as compared to the control for a specific exposure period.

- : The test substance soil loading levels for this study were 1562 mg/Kg, 665mg/Kg, 245mg/Kg, and 97mg/Kg. The control treatment consisted of soil with no test substance. The soil used was artificial, composed of a mixture of 89% sand (>= 50% of the particles between 50 and 200 mm), 1% peat moss (0.5cm sieved to remove coarse fragments) and 10% kaolin clay (96 - 97% kaolinite). The carbon content was 0.37% (2% organic matter). This analysis was not performed in a GLP compliant manner, it is not believed to have affected the results. Fine particles <20 um made up between 13% of the soil (checked by sieving). The artificial soil was not sterilized.

Soil in each loading level and the control was hydrated to 85% of the water holding capacity.

Four replicates were established for each test substance treatment level and control using ten seeds per replicate. Replicate test chambers contained approximately 246g of hydrated soil. Test chambers were glass crystallizing dishes (125 mm X 65 mm).

Mean test temperature: 24.3°C, sd 0.1

Lighting: 16 hour light, 8 hour dark photoperiod. Intensity: 3983 - 4349 Lux

Soil pH: 6.9

Soil depth: 2cm

Test substance

- Organism supplier was Carolina Biological Supply Co., Burlington, NC 27215-3398.
- : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Reliability

- : (1) valid without restriction

Flag

- : Critical study for SIDS endpoint

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(14)

Species

- : Raphanus sativus (Dicotyledon)

Endpoint

- : other: emergence / growth

Exposure period

- : 17 day(s)

Unit

- : mg/kg soil dw

LL50

- : = 1015 measured/nominal

EL50

- : = 446 measured/nominal

Method

- : OECD Guide-line 208 "Terrestrial Plants, Growth Test"

Year

- : 2001

GLP

- : yes

Test substance

- : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

- Method** : The statistical method used to calculate the LL50 values was a maximum likelihood analysis based on Finney, D.J., 1971. Probit Analysis, 3rd Edition, London: Cambridge University Press. The EL50 values were determined using the linear interpolation method (Norberg-King, T.J., A Linear Interpolation Method for Sublethal Toxicity: The Inhibition Concentration (ICp) Approach (Version 2.0). July 1993. U.S. Environmental Protection Agency, Environmental Research Laboratory, Duluth MN).
- Result** : The LL50 (Lethal Loading 50) for Radish (*Raphanus sativus*) = 1015 mg/Kg. The EL50 (Effect Loading 50) for Radish (*Raphanus sativus*) = 446 mg/Kg.
- Test condition** : The LL50 (Lethal Loading 50) is the test substance loading level, which exhibits 50% emergence of the test species as compared to the control for a specific exposure period. The EL50 (Effect Loading 50) is the test substance loading level, which exhibits 50% growth of the test species based on weight as compared to the control for a specific exposure period.
- : The test substance soil loading levels for this study were 1562 mg/Kg, 665mg/Kg, 245mg/Kg, and 97mg/Kg. The control treatment consisted of soil with no test substance. The soil used was artificial, composed of a mixture of 89% sand (>= 50% of the particles between 50 and 200 mm), 1% peat moss (0.5cm sieved to remove coarse fragments) and 10% kaolin clay (96 - 97% kaolinite). The carbon content was 0.37% (2% organic matter). This analysis was not performed in a GLP compliant manner, it is not believed to have affected the results. Fine particles <20 um made up between 13% of the soil (checked by sieving). The artificial soil was not sterilized.
- Soil in each loading level and the control was hydrated to 85% of the water holding capacity.
- Four replicates were established for each test substance treatment level and control using ten seeds per replicate. Replicate test chambers contained approximately 246g of hydrated soil. Test chambers were glass crystallizing dishes (125 mm X 65 mm).
- Mean test temperature: 24.3°C, sd 0.1
Lighting: 16 hour light, 8 hour dark photoperiod. Intensity: 3983 - 4349 Lux
Soil pH: 6.9
Soil depth: 2cm
- Test substance** : Organism supplier was Carolina Biological Supply Co., Bur
: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Reliability Flag** : (1) valid without restriction
: Critical study for SIDS endpoint
- 19.04.2005 (14)
- Species** : *Avena sativa* (Monocotyledon)
Endpoint : other: emergence / growth
Exposure period : 19 day(s)
Unit : mg/kg soil dw
LL50 : = 530 measured/nominal
EL50 : = 225 measured/nominal
Method : OECD Guide-line 208 "Terrestrial Plants, Growth Test"
Year : 2001
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Method** : The statistical method used to calculate the LL50 values was a maximum likelihood analysis based on Finney, D.J., 1971. Probit Analysis, 3rd

Result : Edition, London: Cambridge University Press. The EL50 values were determined using the linear interpolation method (Norberg-King, T.J., A Linear Interpolation Method for Sublethal Toxicity: The Inhibition Concentration (ICp) Approach (Version 2.0). July 1993. U.S. Environmental Protection Agency, Environmental Research Laboratory, Duluth MN).
: The LL50 (Lethal Loading 50) for Oat (*Avena sativa*) = 530 mg/Kg. The EL50 (Effect Loading 50) for Oat (*Avena sativa*) = 225 mg/Kg.

Test condition : The LL50 (Lethal Loading 50) is the test substance loading level, which exhibits 50% emergence of the test species as compared to the control for a specific exposure period. The EL50 (Effect Loading 50) is the test substance loading level, which exhibits 50% growth of the test species based on weight as compared to the control for a specific exposure period.
: The test substance soil loading levels for this study were 1562 mg/Kg, 665mg/Kg, 245mg/Kg, and 97mg/Kg. The control treatment consisted of soil with no test substance. The soil used was artificial, composed of a mixture of 89% sand (>= 50% of the particles between 50 and 200 mm), 1% peat moss (0.5cm sieved to remove coarse fragments) and 10% kaolin clay (96 - 97% kaolinite). The carbon content was 0.37% (2% organic matter). This analysis was not performed in a GLP compliant manner, it is not believed to have affected the results. Fine particles <20 um made up between 13% of the soil (checked by sieving). The artificial soil was not sterilized.

Soil in each loading level and the control was hydrated to 85% of the water holding capacity.

Four replicates were established for each test substance treatment level and control using ten seeds per replicate. Replicate test chambers contained approximately 246g of hydrated soil. Test chambers were glass crystallizing dishes (125 mm X 65 mm).

Mean test temperature: 24.3°C, sd 0.1

Lighting: 16 hour light, 8 hour dark photoperiod. Intensity: 3983 - 4349 Lux

Soil pH: 6.9

Soil depth: 2cm

Test substance : Organism supplier was Carolina Biological Supply Co., Burlington, NC
: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

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

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(14)

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type : artificial soil
Species : other: *Eisenia foetida*
Endpoint : mortality
Exposure period : 14 day(s)
Unit : mg/kg soil dw
LL50 : = 539 measured/nominal
Method : OECD Guide-line 207 "Earthworm, Acute Toxicity Test"
Year : 2001
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Method : The statistical method used to calculate the 7 and 14 day LL50 values for the substance was a maximum likelihood analysis based on Finney, D.J.,

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- Result** : 1971. Probit Analysis, 3rd Edition, London: Cambridge University Press.
: The 7 day LL50 (Lethal Loading 50) was 639mg/Kg with a 95% confidence interval of 560 - 742mg/Kg. The 14 day LL50 was 539mg/Kg with a 95% confidence interval of 451 - 664mg/Kg. These endpoints are based on the mg of test substance per Kg of soil, dry weight.
- Test condition** : The test substance soil loading levels for this study were; 871 mg/kg, 409mg/kg, 203mg/kg, 108mg/kg, and 48mg/kg. The control treatment consisted of soil with no test substance. The soil used was artificial and composed of a mixture of 50% sand (^s 50% of the particles between 50 and 200 mm), 20% kaolin clay (96 - 97% kaolinite) and 30% peat moss (no visible plant material, finely ground).
- Soil in each loading level and the control was hydrated to an overall moisture content of approximately 55% of the dry weight of the artificial soil.
- Four replicates at each loading level were prepared containing 10 worms.
- Test chambers were one quart (approximately 950mL) size glass jars. Jars were approximately 17cm high and approximately 9.5cm in diameter, covered with perforated plastic film to minimize volatility and soil moisture loss.
- Mean test temperature: 18.7°C, sd 0.2
Continuous lighting: 612 - 660 Lux
Soil pH: 6.7
Soil depth: 16cm
- Test substance** : Organism supplier was Carolina Biological Supply Co., Burlington, NC 27215-3398.
: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Reliability Flag** : (1) valid without restriction
: Critical study for SIDS endpoint
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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

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5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type : other: Limit test
Value : > 3160 - mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 3
Vehicle : other: none
Doses : 3160 mg/kg
Method : other: Experimental (Non-regulatory)
Year : 1983
GLP : no
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Result : There were no overt signs of systemic toxicity. Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14. Erythema was noted in all animals at 24 hours, ranging from moderate to severe, and regressed in all animals throughout the study. On Day 14, five of six animals showed very slight erythema and one had no signs of erythema. Edema was evident in all but one animal at 24 hours and by Day 14 all but one animal was free of signs of edema. Desquamation was evident in five animals on Day 14. All animals survived to termination of the study and increased in body weight. There were no significant findings at the postmortem gross examination.

Test condition : Single application / 24-Hour Occlusive Patch
Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Conclusion : C6-C8 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.

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

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

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5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type : other: Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of testing : Bacterial
Test concentration : 50, 100, 200, 400, 600, and 800 µg/plate (50 during repeat assay only; 800 during initial assay only)
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : other: EU Annex V, B.14; OECD 471
Year : 1997
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Result : C6-C8 branched alkyl acetate ester, did not induce significant increases in revertant colonies (> 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains.

Toxicity was observed in the initial assay in the following dose levels and strains: at 100 µg/plate TA1537 (+S9), > 200 µg/plate in TA100 (-S9), TA1535 (+S9), TA1537 (-S9), TA1538 (±S9); > 400 µg/plate in TA98 (±S9), TA1535 (-S9), TA1537 (+S9), and > 600 µg/plate in TA100 (+S9). In the repeat assay, toxicity was observed at doses > 400 µg/plate in TA100 (-S9) and TA1537 (-S9), and at 600 µg/plate in TA98 (-S9), TA1535 (-S9), TA1537 (+S9), and TA1538 (±S9). The nontreated and vehicle controls responded in a manner consistent with data from previous assays.

Test condition : Species/Strain : S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538

Species/cell type: Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9)

Vehicle: DMSO

There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 100, 200, 400, 600, and 800 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control.

Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9.

There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top

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agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 °C for approximately 2 days.

Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.

- Test substance** : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Conclusion** : C6-C8 branched alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested, even at doses that produced evidence of toxicity.
- Reliability Flag** : (1) valid without restriction
19.04.2005 : Critical study for SIDS endpoint (12)
- Type** : other: In Vitro Chromosomal Aberration Assay in CHO Cells
- System of testing** : Cultured Chinese hamster ovary (CHO) cells
- Test concentration** : 80-240 mg/mL in the 20-hour initial test; 40-200 mg/mL in the 20- and 44-hour repeat assays
- Cycotoxic concentr.** :
Metabolic activation : with and without
Result :
Method : other: Galloway, et al, Development of a standard protocol for in vitro cytogenetic testing with Chinese hamster ovary cells: comparison of results for 22 compounds in two laboratories. Environ. Mutagen. 7:1-51, 1985.
- Year** : 1997
- GLP** : yes
- Test substance** : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
- Result** : C6-C8 branched alkyl acetate ester, was tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation. A repeat assay was also performed using 20-hour and 44-hour harvests. For the initial 20-hour harvest data, there was a notable decrease in the percent cell confluency at concentrations ≥ 180 mg/mL with activation and at concentrations ≥ 140 mg/mL without activation. Cell morphology and mitotic indices were acceptable at or below these levels and cell death was prevalent above these levels. For the repeat assay, there were no statistically significant dose-related trends in the percentage of aberrant cells and none of the test concentrations were statistically different than the vehicle control in the 20 or 44 hour activated or nonactivated series. The percentage of aberrant cells in the vehicle control groups ranged from 1% to 2.0%, and the percentage of aberrant cells in the treated groups ranged from 0.0% to 2.6% for the 20 and 44 hour activated and nonactivated series.
- Test condition** : All negative and positive controls used in this study performed in an appropriate manner.
: Treatment group doses (11 total in initial and repeat assays) ranged from 80-240 mg/mL in the 20-hour initial test; 40-200 mg/mL in the 20- and 44-hour repeat assays. S9 activation was used in doses ranging from 80-240 mg/mL in the 20-hour initial assay and ranging from 40-200 mg/mL in the 20- and 44-hour repeat assays. Vehicle in all assays was DMSO (not exceeding 1.0% final volume to ensure normal cell viability and growth rate).
- Positive controls, N-methyl-N-Nitro-N-Nitrosoguanidine (MNNG - clastogen that does not require metabolic activation) and 7,12-Dimethylbenz[a]anthracene (DMBA- clastogen that requires metabolic activation) were used as positive controls in the nonactivated series and activated series, respectively.

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Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Conclusion : C6-C8 branched alkyl acetate ester was considered negative for inducing chromosome aberrations under the conditions of this test at doses up to 180 mg/mL with and 140 mg/mL without metabolic activation.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
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5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

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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

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT