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# I U C L I D

## Data Set

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**Existing Chemical** : ID: 108419-32-5  
**CAS No.** : 108419-32-5  
**TSCA Name** : Acetic acid, C7-9-branched alkyl esters, C8-rich  
**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

**Printing date** : 19.04.2005  
**Revision date** :  
**Date of last update** : 19.04.2005

**Number of pages** : 27

**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

Id 108419-32-5  
Date 19.04.2005

## 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 (CH<sub>3</sub>COOR).  
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

**C7-C9 branched alkyl acetate ester**

18.12.2000

**Exxate 800**

07.06.2004

**oxo-octyl acetate**

07.06.2004

## 1.3 IMPURITIES

# 1. General Information

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## 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

Id 108419-32-5

Date 19.04.2005

### 2.1 MELTING POINT

**Value** : = -30 °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: C8 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** : C8 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 (9)

### 2.2 BOILING POINT

**Value** : = 186 - 215 °C at 1013 hPa  
**Decomposition** :  
**Method** : other: ASTM D1078 Mod  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

**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 (12)

### 2.3 DENSITY

**Type** : relative density  
**Value** : = .87 at 20 °C  
**Method** : other: ASTM D891  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

## 2. Physico-Chemical Data

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**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 (12)

### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

**Value** : = .93 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** : 1999

**GLP** : no data

**Test substance** : other TS: C8 methyl-branched alkyl acetate ester

**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 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** : C8 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 (9)

### 2.5 PARTITION COEFFICIENT

**Partition coefficient** : octanol-water

**Log pow** : = 3.66 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** : 1999

**GLP** : no data

**Test substance** : other TS: C8 methyl-branched alkyl acetate ester

**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. 84:83-92.

**Test substance** : C8 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

## 2. Physico-Chemical Data

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Flag : are calculated and not measured.  
19.04.2005 : Critical study for SIDS endpoint (9)

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water  
Value : = 45 mg/l at 25 °C  
pH value :  
concentration : at °C  
Temperature effects :  
Examine different pol. :  
pKa : at 25 °C  
Description :  
Stable :  
Deg. product :  
Method : other: Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04  
Year : 1999  
GLP : no data  
Test substance : other TS: C8 methyl-branched alkyl acetate ester  
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 : C8 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 (9)

### 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. Physico-Chemical Data

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### 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: C8 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. 108419-32-5; Acetic acid, C7-9 branched alkyl esters, C8-rich  
**Flag** : Critical study for SIDS endpoint  
19.04.2005

**Type** : air  
**Light source** :  
**Light spectrum** : nm  
**Relative intensity** : based on intensity of sunlight

**INDIRECT PHOTOLYSIS**

**Sensitizer** : OH  
**Conc. of sensitizer** : 1500000 molecule/cm<sup>3</sup>  
**Rate constant** : = .000000000000109403 cm<sup>3</sup>/(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: C8 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 <sup>3</sup> /molecule-sec)
11.7	10.94 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** : C8 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 (9)

#### 3.1.2 STABILITY IN WATER

#### 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).

**Result** : Input values used:  
Molecular mass = 172.27 g/mol  
Water solubility = 45 mg/L  
Vapour pressure = 93.3 Pa  
log Kow = 3.66  
Melting point = -30 deg C  
Air- 93.3%  
Water- 1.3%  
Soil- 5.2%  
Sediment - 0.1%  
Suspended Sed - <0.01%

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**Test substance** : Biota - <0.01%  
**Reliability** : CAS No. 108419-32-5; Acetic acid, C7-9 branched alkyl esters, C8-rich  
: (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  
07.06.2004

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#### 3.4 MODE OF DEGRADATION IN ACTUAL USE

#### 3.5 BIODEGRADATION

#### 3.6 BOD5, COD OR BOD5/COD RATIO

#### 3.7 BIOACCUMULATION

**Species** : other: see remark  
**Exposure period** : at °C  
**Concentration** :  
**BCF** : = 151  
**Elimination** :  
**Method** : other: calculation  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: C8 methyl-branched alkyl acetate ester

**Remark** : A log BCF of 2.2 (BCF = 151) is calculated. C8 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)OCCCCC(C)CC

**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  
19.04.2005

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#### 3.8 ADDITIONAL REMARKS

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

**Type** : flow through  
**Species** : Pimephales promelas (Fish, fresh water)  
**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**LC50** : = 14.9 measured/nominal  
**Limit test** : no  
**Analytical monitoring** : yes  
**Method** : other: USEPA 560/6-82-002 Environmental Effects Test Guideline  
**Year** : 1982  
**GLP** : yes  
**Test substance** : other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

**Result** : 96-hour LC50 = 14.9 mg/L (95% CI 9.91 to 20.0) based upon measured TC values.  
 96-hour LL50 = 49.5 % WAF (95% CI 46.26 to 52.97) based upon nominal values.  
 Analytical method used was Total Carbon (TC). TC values represent the mean of samples taken on days 0, 2, and 4 less the control value, which was not reported. The LC50 values based upon TC and were re-calculated in 1994 and issued in an amended report.

Measured Conc. (mg/L of TC)	Fish Total Mortality (@96 hrs)*
Control	0
1.39	0
2.71	0
4.90	0
9.91	0
19.86	20

**Test condition** : \*20 fish added at test initiation  
 Statistical Method: Probit procedure by Litchfield & Wilcoxon  
 A stock water accommodated fraction (WAF) was prepared by adding 267ml of the test substance to ~40L of laboratory blend water in a glass carboy. The solution was stirred for 72 hours and the 100% WAF used for testing. The WAF was administered to the test chambers via a diluter and flow-through delivery system. The diluter system comprised of glass, stainless-steel with no plasticized materials. The diluter prepared the following test treatment levels: control, 4.4, 8.8, 17.5, 35.0, and 70.0 % WAF, which measured NA, 1.39, 2.71, 4.90, 9.91, 19.86 mg/L as Total Carbon (TC). The test chambers were glass culture dishes (150 x 75mm). Two replicates with ten fish each were tested per treatment level. Test temperature was 20.96 +/- 0.15 Deg C. Lighting was gradual on and off with 16 hours dark and 8 hour light with an intensity of 77 to 79 ft candles.  
 Dilution water hardness was 159 mg/L as CaCO<sub>3</sub>.  
 The pH ranged from 7.3 to 8.1. Dissolved Oxygen ranged from 6.7 to 8.4 mg/L.  
 Fish were supplied by in-house laboratory; age = 13 weeks; mean wt.=0.257g; mean total length=2.4cm; test loading=0.21g of fish/L per 24 hour period.

**Reliability** : (2) valid with restrictions  
 Insufficient information in report to assess concentration values.

**Flag** : 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

**Type** : flow through  
**Species** : Daphnia magna (Crustacea)  
**Exposure period** : 48 hour(s)  
**Unit** : mg/l  
**EC50** : = 29.4 measured/nominal  
**Limit Test** : no  
**Analytical monitoring** : yes  
**Method** : other: USEPA TSCA  
**Year** : 1992  
**GLP** : yes  
**Test substance** : other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

**Result** : 48 hour EC50 = 29.4 mg (95% CI 24.6 to 36.3) based upon measured TC values.  
48 hour EC50 = 73.58 % WAF (95% CI 62.18 to 89.3 %) based upon nominal values.

Analytical method used was Total Carbon (TC). Measured TC values are based upon the mean of samples taken on days 0, 1 and 2 less the control value, which was not reported.

Meas. Conc. (mg TC/L)	Daphnia Total Mortality (@48 hrs)*
Control	1
1.87	1
4.13	1
10.24	0
20.21	3
39.95	17

\*20 Daphids total added at test initiation.

Mortality is defined as immobilized.

EC50 based upon TC is the result of a re-calculation in an amended report in 1994.

Statistical Method: Finney, D.J. probit procedure of SAS

**Test condition** : A stock water accommodated fraction (WAF) was prepared by combining test substance with laboratory dilution water, at a ratio of 6.7ml per liter of water. The total volume prepared was not reported. The mixture was stirred for 72 hours and the 100% WAF was drawn out via a siphon tube and used for testing. The WAF was administered to the test chambers via a diluter and flow-through delivery system. The diluter system comprised of glass, stainless steel, with no plasticized materials. The diluter prepared the following test treatment levels: control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF, which measured: NA, 1.87, 4.13, 10.24, 20.21, and 39.95mg /L as Total Carbon (TC). The test chambers were glass tanks with approximately 6L of test solution flowing through over a 24-hour period. Two replicates with ten daphnids each were tested per treatment level.

Test temperature was 21.36 +/- 0.39 Deg. C. Lighting was 16 hours dark and 8 hour light with gradual on/off periods and an intensity of 83 to 87 ft candles.

Dilution water hardness was 157 mg/L measured as CaCO3.

Dissolved oxygen was 7.9 to 8.8mg/L. The pH ranged from 7.5 to 8.1.

**Reliability** : Organisms were supplied by in-house cultures; age = <24 hours old.  
: (2) valid with restrictions  
**Flag** : Insufficient information in report to assess concentration values.  
: Critical study for SIDS endpoint

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### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

**Species** : Selenastrum capricornutum (Algae)  
**Endpoint** : growth rate  
**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**Limit test** : no  
**Analytical monitoring** : yes  
**Method** : other: USEPA, Environmental Effects Test Guideline EPA 560/6-83-002  
**Year** : 1983  
**GLP** : yes  
**Test substance** : other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

**Result** : 72 hour EL50b=20.97mg TC/L (biomass)  
72 hour EL50gr=29.65mg TC/L (growth rate)  
96 hour EL50b=19.4mg TC/L (biomass)  
96 hour EL50gr=43.52mg TC/L (growth rate)

NOELRb = 31.0 mg/L  
NOELRgr = 8.0 mg/L

Analytical method used was Total Carbon (TC). Measured TC values are based upon Day 0 samples minus the control value (3.375mg TC/L). No excursions from the protocol were noted.

Nominal Conc. (%WAF)	Growth Rate		Mean Cell Conc. - 96 hr (cells/ml)
	72 & 96 hr.	(% Inhibition)	
Control	na	na	4.6 x 10(6)
6.25	0.11	1.59	4.0 x 10(6)
12.5	30.24	33.48	2.7 x 10(6)
25.0	2.50	3.33	3.6 x 10(6)
50.0	36.90	34.31	2.5 x 10(6)
100.0	63.51	60.48	1.8 x 10(5)

na - not applicable

**Test condition** : Statistical Method: Inverse interpolation method of Snedecor and Cochran  
A Water Accommodated Fraction (WAF) stock solution was prepared by adding 6.7ml of test substance to 1L of algal nutrient media in a 2L flask and mixed slowly for 72 hours. After mixing, the solution was transferred to a separatory funnel and allowed to settle for one hour. After settling, the solution was removed from the bottom and used as the 100% WAF. Individual treatments were prepared by diluting the 100% WAF with algal nutrient media. The test treatments were divided into 4 replicates. Three replicate were inoculated with algae at  $2.0 \times 10^4$ . The remaining replicate served as a blank. Treatment replicates were 125 ml erlenmeyer flasks containing 50 ml of solution. Flasks were placed on a shaker table during the study at ~100 rpm.  
The test treatment concentrations were; control, 6.25, 12.5, 25, 50 and 100% WAF which measured, NA, 2.78, 5.74, 10.32, 21.46, and 44.71 mg TC/L respectively.

Test temperature was 23.99 Deg. C. Lighting was continuous at ~4300 Lux (400 ft candles). The pH was 7.5 at test initiation and ranged from 7.3 to 7.4 at test termination.

**Reliability** : (3) invalid  
Control TC was 3.3 mg/L instead of the required <2 mg/L.

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### 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. 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  
**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** : yes  
**Test substance** : other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

**Result** : LD50 >3160 mg/kg bw

One animal was sacrificed on Day 11 due to severe weight loss. The surviving five animals showed slight weight gain through the study. Dermal evaluations ranged from no erythema to moderate to severe. Edema scores ranged from no edema to slight edema. Desquamation was noted in four animals during the study. The animal terminated on Day 11 revealed kidney discoloration, small spleen, cecum and ileum, and brown material in the stomach. The remaining five animals showed no abnormalities at necropsy.

**Test condition** : Dermal application. Single application / 24-hour occlusive patch. Post dose observation period 14 days. Number of animals per dose per sex = 3.

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.

**Test substance** : CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

**Conclusion** : C7-C9 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.

**Reliability** : (1) valid without restriction  
No circumstances occurred that would have affected the quality or integrity of the data.

**Flag** : Critical study for SIDS endpoint

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#### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

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### 5.2.1 SKIN IRRITATION

### 5.2.2 EYE IRRITATION

### 5.3 SENSITIZATION

### 5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	90 days
Frequency of treatm.	:	once/day
Post exposure period	:	
Doses	:	0, 0.1, 0.5, and 1.0 g/kg/day
Control group	:	yes
NOAEL	:	= 1000 mg/kg
Method	:	EPA OTS 798.2650
Year	:	1985
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)
Remark	:	13-Week repeated dose oral toxicity (gavage). Volume: < or = 1.111 ml/kg (controls received a dose of water volumetrically comparable to the dosage administered to the high dose group, 1.111 ml/kg).  Clinical laboratory studies (hematology and serum chemistry) were performed pretest on 5 males and 5 females (non-study animals), on 5 animals/sex/dose after 45 days (interim sacrifice), and all animals at study termination. Blood samples were collected from the abdominal aortas following an overnight fast. At 45 days, a complete necropsy was performed and livers were collected, weighed and preserved. After 13 weeks, all surviving animals were weighed, anesthetized and sacrificed by exsanguination. Complete necropsies were performed.
Result	:	Liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and do not indicate toxic effects. Microscopic evaluation of the kidneys revealed evidence of mild tubular nephropathy only in the high-dose male rats that were consistent with alpha-2u-globulin effects.
Conclusion	:	Oral administration of C7-C9 branched alkyl acetate ester daily, 5 days/week for 13 weeks, to rats produced minimal signs of systemic toxicity. There was no treatment-related mortality. The in-life clinical observations were primarily oral and dermal irritation (no clear dose-response). Weekly mean body weights and food consumption values were not significantly altered compared to controls. The qualitative hematologic data were unremarkable at all dose levels for the interim and terminal evaluations. At the terminal sacrifice, there were no biologically significant differences between treated and control animals for the measured clinical chemistries. Terminal liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and not indicative of toxic effects. All other organ weights were comparable to control values. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy only in the high-dose male rats that were

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consistent with alpha-2u-globulin effects. Histopathology review of all other tissues from high-dose animals, including reproductive organs (testes, epididymides, prostate, seminal vesicles, ovaries, uterine horns, cervix, and corpus of the uterus, and vagina), showed normal morphology. The lowest observable effect level was 500 mg/kg. No effects were observed at 100 mg/kg.

**Reliability** : (1) valid without restriction  
No circumstances occurred that affected the quality or integrity of the data.  
**Flag** : Critical study for SIDS endpoint  
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### 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** : 25, 50, 100, 200, 400, and 600 µg/plate (25 repeat assay only; 600 initial assay only)  
**Cycotoxic concentr.** :  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** : EPA OPP 84-2  
**Year** : 1994  
**GLP** : yes  
**Test substance** : other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

**Remark** : Species/Strain - S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538  
Species/cell type - Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9)

**Result** : Vehicle - DMSO  
C7-C9 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.  
In the initial and repeat assay, neither a positive response nor a dose related increase was observed for any of the tester strains. Toxicity, either a reduction in the number of revertant colonies or a reduction in the background lawn, was observed for all five tester strains with an without metabolic activation in both the initial and repeat assays, except for tester strain TA1535 with metabolic activation for the repeat assay. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.

**Test condition** : 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 25, 50, 100, 200, 400, or 600 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-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 agar,

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vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at  $37 \pm 2$  °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. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

**Conclusion** : C7-C9 branched alkyl acetate ester was not mutagenic in any strain of *Salmonella typhimurium* tested.

**Reliability** : (1) valid without restriction  
No circumstances occurred that would have affected the quality or integrity of the data.

**Flag** : Critical study for SIDS endpoint

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### 5.6 GENETIC TOXICITY 'IN VIVO'

**Type** : other: In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method

**Species** : mouse

**Sex** : male/female

**Strain** : other: Crl:CD-1 (VAF/Plus)

**Route of admin.** : gavage

**Exposure period** : 24, 48 and 72 hours

**Doses** : 0.625, 1.25, and 2.5 grams/kg / Single dose

**Result** : negative

**Method** : EPA OTS 798.5395

**Year** : 1994

**GLP** : yes

**Test substance** : other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

**Result** : A statistically significant increase in the mean number of micronucleated polychromatic erythrocytes was not seen at any dose level. Cytotoxicity, shown by a dose-related decrease in the percentage of polychromatic erythrocytes, was observed for both sexes at the 48-hour sampling time (regression coefficient  $p < 0.01$ ). The two highest dose groups were statistically different from the vehicle control. Both the positive (cyclophosphamide) and negative (vehicle carrier) controls responded in an appropriate manner.

The test material is considered to be toxic to bone marrow in CD-1 mice under the conditions of this test based on the decrease in the mean percent of polychromatic erythrocytes at the 48-hour sampling time.

**Test condition** : Vehicle: Corn Oil

Positive Control: Cyclophosphamide (40 mg/kg) in reagent grade water by oral gavage

The test substance and the vehicle were administered as a single dose by oral gavage. The vehicle was dosed at a volume equal to the test substance volume. The positive control was administered as a single dose at a volume equal to the test substance volume. Animals from the appropriate groups were sacrificed at approximately 24, 48, and 72 hours. Animals dosed with Cyclophosphamide were sacrificed at 24 hours only. Immediately following sacrifice, both femurs from each animal were removed and the bone marrow was aspirated, flushed in fetal bovine serum and centrifuged. The cell pellet was resuspended and two slide smears/animal were made. The slides were stained with Acridine Orange and wet mounted. Slides were then evaluated for presence of micronuclei

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**Test substance** : (1000 polychromatic erythrocytes/animal were evaluated).  
CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

**Conclusion** : C7-C9 branched alkyl acetate ester did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-1 mice. Therefore, it is not considered mutagenic under the conditions of this assay.

**Reliability** : (1) valid without restriction  
No circumstances occurred that would have affected the quality or integrity of the data.

**Flag** : Critical study for SIDS endpoint  
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### 5.7 CARCINOGENICITY

#### 5.8.1 TOXICITY TO FERTILITY

#### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

**Species** : rat  
**Sex** : female  
**Strain** : Sprague-Dawley  
**Route of admin.** : gavage  
**Exposure period** : Gravid day 6-15  
**Frequency of treatm.** : single dose daily  
**Duration of test** : Gravid day 20  
**Doses** : 0, 100, 500 and 1000 mg/kg  
**Control group** : other: Sham-Treated with distilled water at 1000 mg/kg  
**NOAEL maternal tox.** : 500 mg/kg bw  
**NOAEL teratogen.** : 500 mg/kg bw  
**other: NOEL Maternal** : 100 mg/kg bw  
**other: NOEL Pup** : 500 - mg/kg bw  
**Method** : EPA OTS 798.4900  
**Year** : 1985  
**GLP** : yes  
**Test substance** : other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

**Remark** : Developmental Toxicity with 22 mated female Sprague-Dawley rats per dose. Vehicle: none.

For the 1000 mg/kg group, there was a slightly increased incidence of malformations, although the different types of malformations, observed did not suggest a characteristic pattern of anomalies. No developmental toxicity was observed at the maternally toxic dose of 500 mg/kg or the maternally nontoxic dose of 100 mg/kg.

Statistical Methods: Maternal body weight, body weight change, food consumption, uterine data (i.e., corpora lutea, implants, resorptions), and malformation data were analyzed with Bartlett's test of homogeneity of variance to determine if groups had equivalent variances at the 15 level of significance. If not significantly different, groups were compared using a one-way standard analysis of variance (ANOVA). If significant differences among means were detected, Duncan's test was used to determine the treated group that differed from control. Fetal weights and crown-rump lengths were analyzed using individual fetal values by a standard nested analysis of variance with values nested within dams and dams nested within groups. If differences within groups were indicated, the least-

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- significant-difference technique was used to determine the group(s) that differed from control. If the groups did not have equivalent variances at the 1% level, then a Kruskal-Wallis test (nonparametric) was used to assess differences in group means. If the means were different, a rank sum comparison was used to determine the treatment group that differed from control.
- Conclusion** : C7-C9 branched alkyl acetate ester, was administered at 0, 100, 500, and 1000 mg/kg on gestation days 6-15 in a developmental toxicity study in rats. Maternal toxicity was seen at the 500 and 1000 mg/kg doses as evidenced by decreases in body weight and food consumption. There was a slight, but not significant increase in fetal malformations and embryotoxicity in the 1000 mg/kg group only; no adverse fetal effects were observed in the 100 and 500 mg/kg groups. (Daughtrey, et al., 1989)
- Reliability** : (1) valid without restriction  
No circumstances occurred that affected the quality or integrity of the data.
- Flag** : Critical study for SIDS endpoint  
19.04.2005 (1) (7)

### 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