

201-14018E

I U C L I D

Data Set

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81977000

Existing Chemical : ID: 108419-33-6
CAS No. : 108419-33-6
TSCA Name : Acetic acid, C8-10-branched alkyl esters, C9-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

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

1. General Information

Id 108419-33-6
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 (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

C8-C10 branched alkyl acetate ester

07.06.2004

Exxate 900

07.06.2004

oxo-nonyl 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 108419-33-6

Date 19.04.2005

2.1 MELTING POINT

Value : = -20 °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
Test substance : other TS: C13 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 : C13 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 (4)

2.2 BOILING POINT

Value : = 205 - 235 °C at 1013 hPa
Decomposition :
Method : other: ASTM D1078 Mod
Year :
GLP : no data
Test substance : other TS

Test substance : CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)

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
07.06.2004 (5)

2.3 DENSITY

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

2. Physico-Chemical Data

Id 108419-33-6

Date 19.04.2005

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
07.06.2004 (5)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .35 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

Test substance : other TS: CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)

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 : CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)

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 (4)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water

Log pow : = 4.15 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

Test substance : other TS: CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)

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 : CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters,

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Reliability : predominantly C9 (>75%)
: (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 (4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 14.5 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
Test substance : other TS: CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)

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. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)

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 (4)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2. Physico-Chemical Data

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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	:	
Test substance	:	other TS: C9 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. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, C9-rich
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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 : = .000000000000123533 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: C9 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)
10.4	12.35 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 : C9 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 (4)

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 = 186.3 g/mol
Water solubility = 14.5 mg/L
Vapour pressure = 34.7 Pa
log Kow = 4.15
Melting point = -20 deg C
Air- 86.7%
Water- 1.0%
Soil- 12.1%
Sediment - 0.3%
Suspended Sed - <0.01%

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Test substance : Biota - <0.01%
Reliability : C9 methyl-branched alkyl acetate ester
: (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 (6)

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 : = 316
Elimination :
Method : other: calculation
Year :
GLP : no data
Test substance : other TS: C9 methyl-branched alkyl acetate ester
Remark : A log BCF of 2.5 (BCF = 316) is calculated. C9 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)OCC(C)CCC(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 (3)

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

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- 4.1 ACUTE/PROLONGED TOXICITY TO FISH
- 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES
- 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE
- 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA
- 4.5.1 CHRONIC TOXICITY TO FISH
- 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES
- 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS
- 4.6.2 TOXICITY TO TERRESTRIAL PLANTS
- 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS
- 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES
- 4.7 BIOLOGICAL EFFECTS MONITORING
- 4.8 BIOTRANSFORMATION AND KINETICS
- 4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : other: Limit
Value : > 5000 mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 5
Vehicle : other: None
Doses :
Method : other: Experimental
Year : 1983
GLP : yes
Test substance : other TS:C8-C10 branched alkyl acetate ester

Remark : There was one female death on day 4 during this study. Nine of 10 animals showed staining in the ano-genital area on Day 1 and all 10 showed staining on Day 2. Hypopnea was observed in 3 rats on Day 1. Other clinical observations included unthrifty coat, hypoactivity, prostration, urinary staining, and soft stool in the first 4 days. Alopecia was observed in one female from Day 10 through 14. All surviving animals showed an increase over pre-dose weights. Five of 9 surviving animals showed no observable abnormalities during postmortem examination. Three animals showed lung discoloration typical of findings resulting from carbon dioxide asphyxiation. The animal that succumbed prior to study termination exhibited vascularization and distension of the cecum; thickened amber material present in the duodenum; thickened red material in the jejunum; an accentuated lobular pattern present in the liver; and, a slightly reddened thymus.

Conclusion : C8-C10 branched alkyl acetate ester elicited minimal signs of acute systemic toxicity when administered orally. Signs of slight toxicity were limited to the first 4 days.

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
 11.12.2001 (2)

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

5. Toxicity

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GLP : yes
Test substance : other TS

Result : LD50 >3160 mg/kg bw

Erythema was noted in all animals at 24 hours and continued in four animals through Day 14. Edema was seen in three animals at 24 hours. No animals showed edema by the Day 7 evaluation. Desquamation was seen in one animal on Day 7, three animals on Day 10 and remained in two animals at the Day 14 termination. One male and two females at Day 7 and one male and one female showed slight decreases in body weight. Food consumption was reduced on Day 1 only. Postmortem examination revealed gallbladder and salivary gland abnormalities, kidney discoloration, a urinary bladder abnormality, hair in two stomachs and ano-genital staining.

Test condition : Dermal Application, Single application / 24-Hour Occlusive Patch, Post Dose Observation Period 14 Days.

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. 108419-33-6, C8-C10 branched alkyl acetate ester
Conclusion : C8-C10 branched alkyl acetate ester has a low order of percutaneous toxicity when administered in a single dose to intact rabbit skin at 3160 mg/kg.

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
02.03.2004

(1)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5. Toxicity

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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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- (1) Bio/dynamics Inc. 1983. Acute Dermal Toxicity Study in the Rabbit with C8-C10 Branched Alkyl Acetate Ester. Project # 330406.
- (2) Bio/dynamics, East Millstone, NJ, Acute Oral Toxicity Study in the Rat; Project # 330401.
- (3) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
- (4) EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
- (5) ExxonMobil Chemical Company (2003). Exxate 900 Data Sheet.
- (6) Mackay D (1998). Level I Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT