

201-15031B1

I U C L I D

Data Set

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Existing Chemical : ID: 1330-61-6
CAS No. : 1330-61-6
EINECS Name : Isodecyl acrylate
EC No. : 215-542-5
TSCA Name : 2-Propenoic acid, isodecyl ester
Molecular Formula : C13H24O2

Producer related part
Company : ACC Specialty Acrylates and Methacrylates Panel
Creation date : 29.11.2001

Substance related part
Company : ACC Specialty Acrylates and Methacrylates Panel
Creation date : 29.11.2001

Status :
Memo : Isodecyl

Printing date : 17.12.2003
Revision date :
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Number of pages : 36

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 1330-61-6
Date 17.12.2003

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

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code : O=C(C=C)OCCCCCCCC(C)C
Molecular formula : C13 H24 O2
Molecular weight : 212.32
Petrol class :

17.12.2003

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : typical for marketed substance
Substance type : organic
Physical status : liquid
Purity : ca. 100 % v/v
Colour : clear
Odour : mild acrylic

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1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Acrylic acid, isodecyl ester
Isodecyl acrylate
Isodecyl alcohol, acrylate
Isodecyl propenoate

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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. General Information

Id 1330-61-6
Date 17.12.2003

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value : = -100 °C
Sublimation :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Handbook data
Rohm and Haas Company Spring House
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
15.12.2003 (4) (7)

Value : = -100 °C
Sublimation :
Method : other: EPIWIN (v3.11) MPBPWIN Submodel (v1.41); experimental database.
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
15.12.2003 (16)

Value : = 11.5 °C
Sublimation :
Method : other: EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); mean of Adapted Joback and Gold & Ogle methods
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
15.12.2003 (16)

Value : = -10.4 °C
Sublimation :
Method : other: EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); mean of Adapted Joback and Gold & Ogle methods
Year : 2003
GLP :
Test substance : other TS

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)
Reliability : (2) valid with restrictions
15.12.2003 (16)

2.2 BOILING POINT

Value : = 158 °C at 66.7 hPa
Decomposition :

2. Physico-Chemical Data

Id 1330-61-6
Date 17.12.2003

Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Handbook data
Rohm and Haas Company Spring House

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
15.12.2003 (7)

Value : = 158 °C at
Decomposition :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Handbook data
Rohm and Haas Company Spring House

Reliability : (2) valid with restrictions
15.12.2003 (4)

Value : = 158 °C at 66.5 hPa
Decomposition :
Method : other: EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); experimental database
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
15.12.2003 (16)

Value : = 253.4 °C at
Decomposition :
Method : other: EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); Adapted Stein and Brown Method
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
15.12.2003 (16)

Value : = 196.8 °C at
Decomposition :
Method : OECD Guide-line 103 "Boiling Point/boiling Range"
Year :
GLP : yes
Test substance : other TS

Remark : IOA polymerises at elevated temperatures
Source : 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)
Reliability : (1) valid without restriction

2. Physico-Chemical Data

Id 1330-61-6
Date 17.12.2003

15.12.2003 (18)

Value : = 216.9 °C at
Decomposition Method :
: other: EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); Adapted Stein and Brown Method
Year : 2003
GLP :
Test substance : other TS

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)
Reliability : (2) valid with restrictions

16.12.2003 (16)

2.3 DENSITY

Type : density
Value : = .885 at 20 °C
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Rohm and Haas Company Spring House
Reliability : (4) not assignable

16.12.2003 (5)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .03 hPa at 25 °C
Decomposition Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Handbook data
Rohm and Haas Company Spring House

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

15.12.2003 (4)

Value : = .03 hPa at 25 °C
Decomposition Method :
: other (calculated): EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); mean VP of Antoine & Grain methods
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions

2. Physico-Chemical Data

Id 1330-61-6

Date 17.12.2003

17.12.2003 (16)

Value : = 1.333 hPa at 25 °C
Decomposition :
Method : OECD Guide-line 104 "Vapour Pressure Curve"
Year :
GLP : yes
Test substance : other TS

Source : 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)

Reliability : (2) valid with restrictions

15.12.2003

Value : = .204 hPa at 25 °C
Decomposition :
Method : other (calculated): EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); mean
VP of Antoine & Grain methods
Year : 2003
GLP :
Test substance : other TS

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)

Reliability : (2) valid with restrictions

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(16)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : = 5.07 at °C
pH value :
Method : other (calculated): EPIWIN (v 3.11); KOWWIN Submodel (v 1.67)
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

15.12.2003

(14)

Partition coefficient :
Log pow : = 5.07 at °C
pH value :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Handbook data
Rohm and Haas Company Spring House

Reliability : (2) valid with restrictions

15.12.2003

(4)

Partition coefficient :
Log pow : = 3.93 at 25 °C

2. Physico-Chemical Data

Id 1330-61-6
Date 17.12.2003

pH value :
Method : other (calculated)
Year :
GLP : no
Test substance : other TS

Remark : The calculated log Pow for IOA agrees well with the measured value for 2-ethylhexyl acrylate, 3.67.

Source : 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)
Reliability : (2) valid with restrictions
16.12.2003 (8)

Partition coefficient :
Log pow : = 4.09 at °C
pH value :
Method : other (calculated): EPIWIN (v 3.11); KOWWIN Submodel (v 1.67)
Year :
GLP :
Test substance : other TS

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)
Reliability : (2) valid with restrictions
15.12.2003 (14)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 1.75 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: EPIWIN (v 3.11); WSKOWWIN Submodel (v 1.41)
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
17.12.2003 (17)

Solubility in :
Value : = 1.75 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

Id 1330-61-6
Date 17.12.2003

Deg. product :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Handbook data
Rohm and Haas Company Spring House

Reliability : (2) valid with restrictions
15.12.2003 (4)

Solubility in : Water
Value : = 12.44 mg/l at 23.1 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : OECD Guide-line 105
Year :
GLP : yes
Test substance : other TS

Source : 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)
Reliability : (1) valid without restriction
15.12.2003 (18)

Solubility in : Water
Value : = 16.8 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: EPIWIN (v 3.11); WSKOWWIN Submodel (v 1.41)
Year : 2003
GLP :
Test substance : other TS

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)
Reliability : (2) valid with restrictions
17.12.2003 (17)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : = 106 °C
Type :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Rohm and Haas Company Spring House
Reliability : (4) not assignable
15.12.2003 (10)

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 : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
DIRECT PHOTOLYSIS
Halflife t1/2 : = .5 day(s)
Degradation : % after
Quantum yield :
Deg. product :
Method : other (calculated): EPIWIN (v 3.11); AOPWIN Submodel (v 1.91)
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Remark : Overall OH rate constant = 22.2E-12 cm³/molecule-sec
 Half-life = 5.8 Hours (12-hr day; 1.5E6 OH/cm³)

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
 17.12.2003 (11)

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
DIRECT PHOTOLYSIS
Halflife t1/2 : = .6 day(s)
Degradation : % after
Quantum yield :
Deg. product :
Method : other (calculated): EPIWIN (v 3.11); AOPWIN Submodel (v 1.91)
Year : 2003
GLP :
Test substance : other TS

Remark : Overall OH rate constant = 19.4E-12 cm³/molecule-sec
 Half-life = 6.6 Hours (12-hr day; 1.5E6 OH/cm³)

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)
Reliability : (2) valid with restrictions
 17.12.2003 (11)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : = 10.6 year at 25 °C
t1/2 pH9 : at °C
t1/2 pH 8 : = 1.1 year at 25 °C
Deg. product :
Method : other (calculated): EPIWIN (v 3.11); HYDROWIN Submodel (v 1.67)
Year : 2003
GLP :

3. Environmental Fate and Pathways

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Test substance : as prescribed by 1.1 - 1.4

Remark : Rate constant: Total Kb for pH>8 at 25 deg C = 2.071E-002
L/mol-sec

Reliability : (2) valid with restrictions
17.12.2003

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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 : other: 1000 kg/hr emission to air
Method : Calculation according Mackay, Level III
Year : 2003

Method : The EPIWIN model was run using the following estimated
physical/chemical properties: Henry's LC: 0.0012 atm-m³/mole; VP:
0.0227 mmHg; and Log Kow: 5.07.

Remark : Level III Fugacity Model (Full-Output):

=====
Chem Name: 2-Propenoic acid, isodecyl ester
Molecular Wt: 212.34
Henry's LC: 0.0012 atm-m³/mole (Henrywin program)
Vapor Press: 0.0227 mm Hg (Mpbpwin program)
Log Kow: 5.07 (Kowwin program)
Soil Koc: 4.82e+004 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	96.3	10.8	1000
Water	1.58	360	0
Soil	1.05	360	0
Sediment	1.03	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.54e-011	865	134	86.5	13.4
Water	5.77e-012	0.424	0.22	0.0424	0.022
Soil	3.97e-014	0.281	0	0.0281	0
Sediment	1.74e-012	0.0687	0.00286	0.00687	0.000286

Persistence Time: 13.9 hr

Reaction Time: 16.1 hr

3. Environmental Fate and Pathways

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Advection Time: 104 hr
Percent Reacted: 86.6
Percent Advected: 13.4

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 10.75
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.870 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Result : Concentration (%):
Air = 96
Water = 1.6
Soil = 1.1
Sediment = 1.0

Test substance : as prescribed by 1.1 - 1.4
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
17.12.2003

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Media : other: 1000 kg/hr emission to water
Method : Calculation according Mackay, Level III
Year : 2003

Method : The EPIWIN model was run using the following estimated physical/chemical properties: Henry's LC: 0.0012 atm-m³/mole; VP: 0.0227 mmHg; and Log Kow: 5.07.

Remark : Level III Fugacity Model (Full-Output):

=====
Chem Name: 2-Propenoic acid, isodecyl ester
Molecular Wt: 212.34
Henry's LC: 0.0012 atm-m³/mole (Henrywin program)
Vapor Press: 0.0227 mm Hg (Mppbpwin program)
Log Kow: 5.07 (Kowwin program)
Soil Koc: 4.82e+004 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.54	10.8	0
Water	59.7	360	1000
Soil	0.0168	360	0
Sediment	38.7	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	5.75e-012	322	49.9	32.2	4.99
Water	5.06e-009	372	193	37.2	19.3
Soil	1.48e-014	0.105	0	0.0105	0
Sediment	1.53e-009	60.4	2.51	6.04	0.251

Persistence Time: 324 hr
Reaction Time: 429 hr

3. Environmental Fate and Pathways

Id 1330-61-6
Date 17.12.2003

Advection Time: 1.32e+003 hr
Percent Reacted: 75.4
Percent Advected: 24.6

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 10.75
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.870 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Result : Concentration (%):
Air = 1.5
Water = 60
Soil < 0.1
Sediment = 39

Test substance Reliability : as prescribed by 1.1 - 1.4
17.12.2003 : (2) valid with restrictions

(15)

Media Method Year : other: 1000 kg/hr emission to air
: Calculation according Mackay, Level III
: 2003

Method : The EPIWIN model was run using the following estimated physical/chemical properties: Henry's LC: 0.0006 atm-m³/mole; VP: 0.153 mmHg; and Log Kow: 4.09.

Remark : Level III Fugacity Model (Full-Output):

=====
Chem Name: 2-Propenoic acid, isooctyl ester
Molecular Wt: 184.28
Henry's LC: 0.0006 atm-m³/mole (Henrywin program)
Vapor Press: 0.153 mm Hg (Mppbwin program)
Log Kow: 4.09 (Kowwin program)
Soil Koc: 5.04e+003 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	95.7	12.2	1000
Water	2.94	360	0
Soil	1.09	360	0
Sediment	0.231	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.98e-011	849	149	84.9	14.9
Water	7.41e-012	0.883	0.459	0.0883	0.0459
Soil	2.53e-013	0.327	0	0.0327	0
Sediment	2.4e-012	0.0173	0.00072	0.00173	7.2e-005

Persistence Time: 15.6 hr
Reaction Time: 18.4 hr
Advection Time: 104 hr

3. Environmental Fate and Pathways

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Percent Reacted: 85
Percent Advected: 15

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 12.2
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.932 (weeks)

Advection Times (hr):

Air: 100
Water: 1000
Sediment: 5e+004

Result : Concentration (%):

Air = 96
Water = 2.9
Soil = 1.1
Sediment < 1.0

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)

Reliability : (2) valid with restrictions

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Media : other: 1000 kg/hr emission to water

Method : Calculation according Mackay, Level III

Year : 2003

Method : The EPIWIN model was run using the following estimated physical/chemical properties: Henry's LC: 0.0006 atm-m³/mole; VP: 0.153 mmHg; and Log Kow: 4.09.

Remark : Level III Fugacity Model (Full-Output):

=====

Chem Name: 2-Propenoic acid, isooctyl ester
Molecular Wt: 184.28
Henry's LC: 0.0006 atm-m³/mole (Henrywin program)
Vapor Press: 0.153 mm Hg (Mppbwin program)
Log Kow: 4.09 (Kowwin program)
Soil Koc: 5.04e+003 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.38	12.2	0
Water	90.5	360	1000
Soil	0.027	360	0
Sediment	7.1	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	7.38e-012	316	55.7	31.6	5.57
Water	3.42e-009	408	212	40.8	21.2
Soil	9.43e-014	0.122	0	0.0122	0
Sediment	1.11e-009	7.99	0.332	0.799	0.0332

Persistence Time: 234 hr
Reaction Time: 320 hr
Advection Time: 874 hr
Percent Reacted: 73.2

Percent Advected: 26.8

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 12.2
 Water: 360
 Soil: 360
 Sediment: 1440
 Biowin estimate: 2.932 (weeks)

Advection Times (hr):

Air: 100
 Water: 1000
 Sediment: 5e+004

Result : Concentration (%):
 Air = 2.4
 Water = 91
 Soil < 0.1
 Sediment = 7.1

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)

Reliability : (2) valid with restrictions
 17.12.2003

(15)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic
Contact time : 28 day(s)
Degradation : = 100 (±) % after 28 day(s)
Result : readily biodegradable
Kinetic of testsubst. : 5 day(s) = 72 %
 15 day(s) = 100 %
 %
 %
 %

Deg. product :
Method : OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year :
GLP : no
Test substance : other TS: 2-Propenoic acid, isooctyl ester, Lot 1023, containing 10-15 ppm methylethylhydroquinone

Remark : The sodium benzoate reference solution showed dissolved oxygen losses of 56, 74 and >83% at 5, 15 and 28 days, respectively.

Average loss of IOA in the uninhibited samples was 72% after 5 days. Loss after 15 and 28 days was 100% at each of the concentrations (concentrations not mentioned). Dissolved oxygen levels declined in proportion to IOA levels.

In the inhibited samples, loss of IOA was 0.4, 30 and 6.9% at 5, 15 and 28 days, respectively, with no oxygen

3. Environmental Fate and Pathways

Id 1330-61-6
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Source : depletion.
: 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
15.12.2003 (18)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : other: laboratory test, no data on water renewal
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : = .34
LC50 : = .67
Limit test :
Analytical monitoring : yes
Method : OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year :
GLP : yes
Test substance : other TS

Source : 3M Belgium B.V. Zwijndrecht
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test condition : Test species: Juvenile fathead minnows, mean length 1.6 cm.
Test substance : Isooctyl acrylate (CAS No. 29590-42-9)
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
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Type :
Species : other: fish
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = .9 calculated
Method : other: EPIWIN (v 3.11); ECOSAR Submodel (v 0.99g)
Year :
GLP :
Test substance :

Test substance : as prescribed by 1.1 - 1.4
Reliability : (2) valid with restrictions
 17.12.2003 (12)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
NOEC : < .24
EC50 : = .4
Analytical monitoring : yes
Method : OECD Guide-line 202
Year :
GLP : yes
Test substance : other TS

Remark : Based on the initial measured concentrations, 48-h EC50 and NOEC values for Daphnia magna as determined from the acute

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immobilisation test were 0.77 mg/l and <0.56 mg/l, respectively.

Similarly, its 48-h EC50 and NOEC values, based on mean measured concentrations, were 0.40 mg/l and <0.24 mg/l, respectively.

Source : 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test condition : Test species: Daphnia magna, less than 24-h old neonates.

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)
Lot number 1419

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

17.12.2003

(18)

Type :

Species : other: Daphnid

Exposure period : 48 hour(s)

Unit : mg/l

EC50 : = .55 calculated

Method : other: EPIWIN (v 3.11); ECOSAR Submodel (v 0.99g)

Year :

GLP :

Test substance :

Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions

17.12.2003

(12)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species :

Endpoint : growth rate

Exposure period : 96 hour(s)

Unit : mg/l

NOEC : = 1.7

EC50 : = 2.13

Limit test :

Analytical monitoring : no data

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

Year :

GLP : yes

Test substance : other TS

Source : 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

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(18)

Species : other algae: Green algae

Endpoint :

Exposure period : 96 hour(s)

Unit : mg/l

EC50 : = .066 calculated

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Id 1330-61-6
Date 17.12.2003

Method : other: EPIWIN (v 3.11); ECOSAR Submodel (v 0.99g)
Year :
GLP :
Test substance :

Test substance : as prescribed by 1.1 - 1.4
Reliability : (2) valid with restrictions
17.12.2003

(12)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species : Daphnia magna (Crustacea)
Endpoint : reproduction rate
Exposure period : 14 day(s)
Unit : mg/l
NOEC : = .51
EC50 : = 1.99
IC50 : = .97
Analytical monitoring : yes
Method : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year :
GLP : yes
Test substance : other TS

Result : The results mentioned above were based on mean measured concentrations.

Based on initial measured concentrations:

NOEC = 0.79 mg/l
EC50 = 2.93 mg/l
IC50 = 1.50 mg/l

Source : 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test condition : Test species: Daphnia magna (Crustacea), less than 24-h old neonates
Test substance : 2-Propenoic acid, isoctyl ester (lot 3290)
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

17.12.2003

(18)

Species : Daphnia magna (Crustacea)
Endpoint : reproduction rate
Exposure period : 21 day(s)
Unit : mg/l
NOEC : < .13
EC50 : = 1.61
IC50 : = 1.02
Analytical monitoring : yes
Method : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"

4. Ecotoxicity

Id 1330-61-6
Date 17.12.2003

Year :
GLP : yes
Test substance : other TS

Result : The results mentioned above were based on mean measured concentrations.

Based on initial measured concentrations:

NOEC < 0.20 mg/l
EC50 = 2.62 mg/l
IC50 = 1.72 mg/l

Source : 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test condition : Test species: Daphnia magna (Crustacea), less than 24-h old neonates
Test substance : 2-Propenoic acid, isoocetyl ester (CAS No. 29590-42-9)
Lot 3290

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
17.12.2003 (18)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION**5.1.1 ACUTE ORAL TOXICITY**

Type : LD50
Value : > 5000 mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 10
Vehicle :
Doses : 5000 mg/kg bw
Method : OECD Guide-line 401 "Acute Oral Toxicity"
Year : 1989
GLP : yes
Test substance : other TS

Method : Test method: limit test
 Five male and five female young adult albino rats, weighing between 228 and 288 g were fasted overnight and administered undiluted IOA monomer at a dose of 5000 mg/kg body weight by oral gavage. The animals were housed by sex in groups of five. The animals were observed for clinical signs and mortality for 1, 2.5 and 4 hours post-dosing, then daily for the 14 days following dosing, at which time they were sacrificed, weighed and subjected to gross necropsy.

Result : No treatment-related mortality occurred during the study. Average body weights for male and female rats increased by 43 and 13%, respectively, over the course of the study. Clinical signs consistent with gastrointestinal irritation (diarrhea) and mild central nervous system depression (ataxia and hypoactivity) were observed in most of the animals for the first two days after dosing. No significant gross lesions were noted at necropsy.

Source : 3M Belgium B.V. Zwijndrecht
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test condition : Temperature and humidity of the animal room ranged from 18 to 23 degrees C and from 19 to 39%, respectively.

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

17.12.2003

(1) (2)

5.1.2 ACUTE INHALATION TOXICITY**5.1.3 ACUTE DERMAL TOXICITY****5.1.4 ACUTE TOXICITY, OTHER ROUTES**

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	dermal
Exposure period	:	6-8 weeks
Frequency of treatm.	:	daily
Post exposure period	:	not applicable
Doses	:	Phase I: 0, 1.0, 7.5 and 15%; Phase II: 0 and 25% (lowered to 20% after one week)
Control group	:	yes, concurrent vehicle
NOAEL	:	= 15 %
LOAEL	:	= 20 - %
Method	:	other: OECD Guideline 422
Year	:	1993
GLP	:	yes
Test substance	:	other TS

Method : The study was conducted in two phases. Phase I evaluated the 1.0, 7.5 and 15% concentrations with the first control group and the second phase examined the 25/20% group with the second control group. The second phase was conducted due to a lack of effects in Phase I. Animals received daily dermal applications of IOA in acetone at a constant dose volume of 100 ul/day. In Phase II, marked irritation at the treatment site in the high dose group after one week of dosing was observed and, the IOA concentration for this group was lowered to 20% and the treatment site was moved to an adjacent area for the remainder of the study. The control groups were dosed similarly with 100 ul of acetone. The dermal route of exposure was used because it is the most likely route of occupational exposure.

Each animal was dosed with the test solution for at least six hours/day for two weeks before mating and throughout mating until sacrifice at post-natal day 4. The fur was clipped from the dorsal intrascapular area of the trunk before initiation of treatment and as needed thereafter. The second treatment site for the high dose group was on the posterior portion of the dorsal surface. The dose was spread uniformly over the treatment site and a collar was applied for approximately six hours to avoid ingestion. During the exposure period, animals were singly housed; i.e. mating pairs were separated and pups removed from nesting cages.

Dosing solutions were prepared in acetone. Homogeneity and stability of the Isooctyl Acrylate in the acetone solutions was confirmed prior to the start of the study. Dosing solution concentrations were confirmed

throughout the study.

The animals were observed twice daily for mortality, moribundity, and signs of poor health or abnormal behavior as well as for signs of abnormal pregnancy for females during gestation.

Dermal irritation was scored for each animal before each application of the test material or carrier (except on Day 0) and on the day of necropsy. Because of the change in dose level and dose site for Group 6, both sites were scored daily. Females that were observed in the process of delivering at the time of dermal scoring were not scored on that day.

Individual body weight data for males were recorded on the first day of treatment, weekly thereafter, and on the day of necropsy. Females were weighed on the first day of treatment, weekly during pre-mating, on presumed gestation days (gd) 0, 7, 14 and 20, on lactation days 0 and 4, and on the day of necropsy. Females that did not show positive mating were weighed weekly and on the day of sacrifice.

Individual food consumption data were recorded weekly during the pre-mating phase. Food consumption was measured for mated females for presumed gd 0-7, 7-14 and 14-20 and for females that delivered litters for lactation days 0-4.

Hematology and clinical chemistry measurements were made for all adult males before sacrifice. The animals were fasted overnight prior to blood collection. The following hematology parameters were evaluated: RBC, hemoglobin, hematocrit, platelet count, WBC, MCH, MCHC, MCV, differential blood cell count and blood cell morphology. The following clinical chemistry measurements were made: glucose, urea, nitrogen, creatinine, total protein, albumin, globulin, total bilirubin, cholesterol, AST, ALT, GGT, calcium, inorganic phosphorus, sodium, potassium and chloride.

After removal and sacrifice of the pups, the parental animals were weighed and sacrificed. Females that did not deliver were sacrificed on presumed gd 26. A complete necropsy was performed for all adults. Uteri and ovaries were examined for implantations and corpora lutea. Uteri that appeared non-gravid were stained for confirmation of pregnancy. The following organs were weighed: epididymides, kidneys, liver, testes and thymus. The following tissues were preserved and examined histologically: adrenals, brain, heart, epididymides, kidneys, liver, ovaries, skin (treated and untreated), spleen, testes and grossly observed lesions.

Statistical Analyses: Levene's test was done to test for variance homogeneity. Transformation was used to stabilize the variance when homogeneity was not met. Analysis of variance [ANOVA] was done on the homogeneous or transformed data. If the ANOVA was significant, Dunnett's t-test was used for pairwise comparisons between groups. When no transformation established variance homogeneity at $p < 0.001$, the data were also examined by nonparametric techniques using the Wilcoxon-Mann-Whitney two-sample rank test. One-way ANOVA was used to analyze continuous data such as body weights, body weight changes, food consumption, clinical chemistry and hematology values (except red blood cell morphology).

Result

: There were no test material-related clinical observations or adverse effects on body weights, body weight changes or food consumption. In Phase I (0,

1.0, 7.5 and 15%), a brownish-orange discoloration of the skin at the dosing site was observed for both sexes in all dose groups in a non-dose-related manner. Only minimal skin irritation in a few animals was observed inconsistently during the study through Day 54. Due to the lack of a clear treatment-related effect, Phase II (0 and 25/20%) was conducted. During the first week of dosing at 25% IOA, slight to moderate erythema, edema, desquamation and fissuring were observed in both sexes. In addition, two males were observed with subcutaneous hemorrhage. Because of this irritation, the dose concentration was reduced to 20% for the remainder of the study and was applied to a different location on each animal. Overall, dermal irritation was noted in the high dose group and included slight to moderate erythema and slight desquamation for males and slight erythema, slight to moderate desquamation and slight fissuring for females. Minimally higher serum aspartate aminotransferase and alanine aminotransferase levels were noted in males in the high dose group. There were no significant differences from controls in terminal body weights, absolute organ weights, organ-to-body weight percentages or macroscopic or microscopic findings for any dose group.

Mean measured test concentrations during the 8-week study ranged from 97 to 112% of the nominal concentrations.

See also section 5.8

Source : 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : 2-Propenoic Acid, Isooctyl Ester, IOA (CAS No. 29590-42-9); Purity: 99.75%

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

17.12.2003 (3)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test

System of testing : S. typhimurium TA1535, TA1537, TA1538, TA98 and TA100

Test concentration : Six concentrations ranging from 0.005 to 0.5 ul/plate

Cytotoxic concentr. : 5.0 ul/plate

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 471

Year : 1980

GLP : no

Test substance : other TS

Method : The assay was performed with and without Aroclor 1254-induced rat liver S9 homogenate (approx. 15 mg protein/plate) as a metabolic activation system. Tests were run in quadruplicate with six concentrations of IOA ranging from 0.005 to 0.5 ul/plate. These concentrations were selected on the basis of a preliminary toxicity range-finding study in which IOA was toxic to strain TA100 at a concentration of 5.0 ul/plate but not at concentrations ranging from 0.01 to 1.0 ul/plate. Dimethylsulfoxide (DMSO) was used as the solvent control for all test strains. Positive controls were 2-anthramine (all strains), sodium azide (TA1535 and TA100), 9-aminoacridine (TA1537) and 2-nitrofluorene (TA1538 and TA98).

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- Remark** : This test was performed at SRI International, Menlo Park, CA, USA, beginning in May 1980. Although the study was not conducted according to GLPs, any deviation from current practice is believed not to have materially influenced the overall findings of the study.
- Result** : The highest IOA concentration tested, 0.5 ul/plate, produced pinpoint colonies, indicating toxicity, in strain TA100. The positive controls showed significant (greater than two-fold) increases in the number of revertant colonies per plate compared to the DMSO negative control. No significant increase in revertants was observed at any IOA concentration, either with or without metabolic activation. IOA was not mutagenic under the conditions of the study.
- Source** : 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
- Test substance** : Isooctyl acrylate (CAS No. 29590-42-9); Purity: not stated.
- Reliability** : (1) valid without restriction
- Flag** : Critical study for SIDS endpoint
- 17.12.2003 (2) (9)
- Type** : Mouse lymphoma assay
- System of testing** : Mouse lymphoma cells, L5178Y TK+/-
- Test concentration** : 10 concentrations ranging from 0.0015 to 0.11 ul/ml
- Cycotoxic concentr.** :
- Metabolic activation** : with and without
- Result** : negative
- Method** : OECD Guide-line 476
- Year** : 1980
- GLP** : yes
- Test substance** : other TS
- Method** : IOA monomer was evaluated for mutagenic activity in L5178Y TK+/- mouse lymphoma cells according to a modification of the method of Clive [Mutat. Res. 31, 17 (1975)]. The assay was performed with and without Aroclor 1254-induced rat liver S9 homogenate as the metabolic activation system. Triplicate tests were run with 10 concentrations of IOA ranging from 0.0015 to 0.02 ul/ml without activation and 0.0084 to 0.11 ul/ml with activation. These concentrations were selected on the basis of preliminary toxicity range finding studies. Dimethylsulfoxide (DMSO) was used as the solvent and negative control. Ethylmethanesulfonate (EMS) and 7,12-dimethylbenz(a)anthracene (DMBA) were positive controls for the nonactivated and activated cultures, respectively.
- Remark** : This test was performed at EG&G Mason Research Institute, Rockville, MD, USA, beginning in May 1980.
- Result** : Average cloning efficiencies of the DMSO negative controls were 75.8 and 76.2% for the nonactivated and activated cultures, respectively. Average suspension growth factors for the DMSO negative controls were 20.7 and 11.1 for the nonactivated and activated cultures, respectively. Suspension growth for the nonactivated IOA cultures ranged from 19 to 98% and for the activated IOA cultures from 23 to 124%. The lowest concentration producing cell toxicity was 0.063 ul/ml in cultures with metabolic activation and 0.0036 ul/ml in cultures without metabolic activation. The positive controls showed significant (greater than two-fold) increases in mutant frequency compared to the DMSO negative control. With metabolic activation, three IOA concentrations had mutant frequencies which were two-fold greater than the solvent control but these were considered to be within the range of experimental error. Dose-related increases in mutant frequencies were not observed in either the activated or nonactivated portions of the assay. IOA was not mutagenic under the conditions of the

Source : assay.
 : 3M Belgium B.V. Zwijndrecht
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : Isooctyl acrylate (CAS No. 29590-42-9); Purity: not stated.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
 17.12.2003 (2) (6)

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

Type : other
In vitro/in vivo :
Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : dermal
Exposure period : 6-8 weeks
Frequency of treatm. : Daily
Duration of test : 56 Days
Doses : Phase I: 0, 1.0, 7.5 and 15%; Phase II: 0 and 25% (lowered to 20% after one week)
Control group : yes, concurrent vehicle
Method : other: OECD Guideline 422
Year : 1993
GLP : yes
Test substance : other TS

Method : The study was conducted in two phases. Phase I evaluated the 1.0, 7.5 and 15% concentrations with the first control group and the second phase examined the 25/20% group with the second control group. The second phase was conducted due to a lack of effects in Phase I. Animals received daily dermal applications of IOA in acetone at a constant dose volume of 100 ul/day. In Phase II, marked irritation at the treatment site in the high dose group after one week of dosing was observed and, the IOA concentration for this group was lowered to 20% and the treatment site was moved to an adjacent area for the remainder of the study. The control groups were dosed similarly with 100 ul of acetone. The dermal route of exposure was used because it is the most likely route of occupational exposure.

Each animal was dosed with the test solution for at least six hours/day for

two weeks before mating and throughout mating until sacrifice at post-natal day 4. The fur was clipped from the dorsal intrascapular area of the trunk before initiation of treatment and as needed thereafter. The second treatment site for the high dose group was on the posterior portion of the dorsal surface. The dose was spread uniformly over the treatment site and a collar was applied for approximately six hours to avoid ingestion. During the exposure period, animals were singly housed; i.e. mating pairs were separated and pups removed from nesting cages.

Dosing solutions were prepared in acetone. Homogeneity and stability of the Isooctyl Acrylate in the acetone solutions was confirmed prior to the start of the study. Dosing solution concentrations were confirmed throughout the study.

The animals were observed twice daily for mortality, moribundity, and signs of poor health or abnormal behavior as well as for signs of abnormal pregnancy for females during gestation.

Pairing was initiated after 14 days of dosing. Each female was paired with one male from the same group for a maximum of 14 days. Vaginal examinations were done daily during cohabitation, and the presence of sperm in the vaginal smear or a copulatory plug was considered evidence of positive mating. The day when such evidence was noted was designated gd 0. When mating was confirmed, the males and females were separated. Females that did not show evidence of mating were placed in nesting boxes after completion of the 2-week mating period.

Litter observations: On postnatal day (pnd) 0, the sex of each pup was determined and litter size was recorded. Each live pup was examined for external abnormalities and weighed. On pnd 4, the sex of each pup was determined and the litter size recorded. The pups were examined for external abnormalities and weighed individually before sacrifice. Following sacrifice, the pups were examined for cervical, thoracic or abdominal visceral abnormalities and then discarded. Abnormal tissues were preserved. Whenever possible, dead pups were examined for cervical, thoracic and abdominal visceral abnormalities and congenital abnormalities, then discarded.

After removal and sacrifice of the pups, the parental animals were weighed and sacrificed. Females that did not deliver were sacrificed on presumed gd 26. A complete necropsy was performed for all adults. Uteri and ovaries were examined for implantations and corpora lutea. Uteri that appeared non-gravid were stained for confirmation of pregnancy. The following organs were weighed: epididymides, kidneys, liver, testes and thymus. The following tissues were preserved and examined histologically: adrenals, brain, heart, epididymides, kidneys, liver, ovaries, skin (treated and untreated), spleen, testes and grossly observed lesions.

Statistical Analyses: Levene's test was done to test for variance homogeneity. Transformation was used to stabilize the variance when homogeneity was not met. Analysis of variance [ANOVA] was done on the homogeneous or transformed data. If the ANOVA was significant, Dunnett's t-test was used for pairwise comparisons between groups. When no transformation established variance homogeneity at $p < 0.001$, the data were also examined by nonparametric techniques using the Wilcoxon-Mann-Whitney two-sample rank test. One-way ANOVA was used to analyze continuous data such as body weights, body weight changes, food

- consumption, clinical chemistry and hematology values (except red blood cell morphology), litter data and length of gestation. Reproduction indices (number inseminated, number pregnant, female fertility and gestation index) were analyzed by the Cochran-Armitage test for trend and departure and by a Fisher-Irwin exact test. One-way analysis of covariance was used to analyze the pup body width with the number of pups in the litter as the covariate. Groups were compared to their respective control group for Phases I and II.
- Result** : There were no test material-related clinical observations or adverse effects on body weights, body weight changes or food consumption. In Phase I (0, 1.0, 7.5 and 15%), a brownish-orange discoloration of the skin at the dosing site was observed for both sexes in all dose groups in a non-dose-related manner. Only minimal skin irritation in a few animals was observed inconsistently during the study through Day 54. Due to the lack of a clear treatment-related effect, Phase II (0 and 25/20%) was conducted. During the first week of dosing at 25% IOA, slight to moderate erythema, edema, desquamation and fissuring were observed in both sexes. In addition, two males were observed with subcutaneous hemorrhage. Because of this irritation, the dose concentration was reduced to 20% for the remainder of the study and was applied to a different location on each animal. Overall, dermal irritation was noted in the high dose group and included slight to moderate erythema and slight desquamation for males and slight erythema, slight to moderate desquamation and slight fissuring for females.
- There were no treatment-related effects on male fertility, female fertility, mean days to mating, length of gestation, gestation length, pup viability, mean number of pups/litter or pup weights. There were no treatment-related findings at necropsy of the pups. Reproductive organ weight and histopathology findings for the adults were similar to controls. The reproductive and developmental NOAEL was 20%.
- Source** : 3M Belgium B.V. Zwijndrecht
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
- Test substance** : 2-Propenoic Acid, Isooctyl Ester, IOA (CAS No. 29590-42-9); Purity: 99.75%
- Reliability** : (1) valid without restriction
- Flag** : Critical study for SIDS endpoint
- 17.12.2003 (3)

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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- (12) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; ECOSAR Version 0.99g; PC-Computer software developed by ECOSAR Program, Risk Assessment Division (7403), Washington, D.C.
- (13) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; HYDROWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

9. References

Id 1330-61-6

Date 17.12.2003

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-15031B2

OECD Screening Information Data Sets (SIDS)

Screening Information Data Set
SIDS for High Production Volume Chemicals

Organisation for Economic Co-operation and Development

OECD Initial Assessment

Processed by IRPTC

International Register of Potentially Toxic Chemicals

VOLUME 1
part 2

A Contribution To IPCS
International Programme of Chemical Safety

February 1995

	Substance
Chemical Name	: 2-Propenoic acid, isooctyl ester
Common Name	: Isooctyl acrylate
CAS Number	: 29590-42-9

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End Point : IDENTIFIERS, PHYSICAL AND CHEMICAL
PROPERTIES

Chemical Name : 2-Propenoic acid, isooctyl ester

Common Name : Isooctyl acrylate

CAS Number : 29590-42-9

Synonyms

Acrylic acid, isooctyl ester IOA

Properties & Definitions

Molecular Formula : C₁₁H₂₀O₂

Molecular Weight : 184.2

Boiling Point : 196.8C

State : liquid

Flash Point : 91.0C

Density : 0.88

Vapour Pressure : 0.1333kPa (1.0mmHg) at 25C*

Octanol/Water Partition : log Pow = 3.93 at 25C

Coefficient

Water Solubility : 12.44mg/l at 23.1C

Colour : Colourless

Additives : Methylenehydroquinone (MEHQ) may be used as stabilizer at concentrations up to 20ppm.

Impurities : 2-Propenoic acid, isononyl esters 3.16% (w/w), 2-propenoic acid, isoheptyl esters 1.62% (w/w), acrylate/acrylic acid adducts 0.45 (w/w), isooctyl alcohol 0.32% (w/w), 2-propenoic acid,

isodecyl esters 0.05% (w/w), 2-propenoic acid, isohexyl esters 0.02 (w/w).

General Comments : IOA polymerizes at elevated temperatures. *VP = 0.33kPa (2.5mmHg) at 50C is also reported. The calculated log Pow for IOA agrees well with the measured value for 2-ethylhexyl acrylate 367. Viscosity: 2cps. Reactivity: violent, polymerization may result on exposure to heat.

Overall Evaluation

EXPOSURE

General discussion: IOA is manufactured in the U.S. by a single company (3M, St. Paul, MN) as an intermediate used for the synthesis of acrylic polymers. IOA monomer is not sold commercially. One product containing unreacted IOA as a component is sold by 3M as a concrete sealer for use by professional tradespeople. The IOA monomer in this product, about 1000kg/year, is polymerized at the job site. Trace amounts of unreacted IOA (typically less than 0.1% by weight) are present in certain industrial and consumer products (e.g. adhesive tapes) sold by 3M.

Environmental exposure: waste monomer is incinerated in a hazardous waste incinerator. There is no intentional discharge to water. Airborne emissions from 3M facilities are less than 1ppm (the limit of detection) for expected worst case operations. Industrial and consumer products containing trace amounts of unreacted IOA may be landfilled or incinerated after use. IOA is rapidly biodegraded aerobically and is expected to be rapidly oxidized in the atmosphere.

Consumer exposure: there are no known consumer uses for IOA monomer. Trace residual amounts of unreacted IOA (typically less than 0.1% by weight) are present in certain consumer products sold by 3M.

Occupational exposure: approximately 200 3M employees work in areas in which exposure to IOA, either as the liquid or vapor, may occur. Certain processes involving IOA are open systems in which IOA vapor may be generated. Ventilation systems are used to keep IOA vapor concentrations below the 3M Exposure Guideline of 5ppm (8-hour TWA). This guideline was established in 1981 and is based on the TLV established by the ACGIH for ethyl acrylate. Air monitoring studies of 3M processing and manufacturing areas have typically indicated

airborne IOA concentrations to be less than 1ppm. impermeable gloves are required to be worn by all employees who may come into contact with unreacted IOA monomer.

TOXICITY

Human toxicity: on acute exposure, IOA is practically non-toxic orally to rats and is slightly irritating to the eyes and skin of rabbits.

IOA is expected to be a weak skin sensitizer by analogy to other low molecular weight acrylate esters. Repeated dermal exposure to IOA caused no systemic toxicity or reproductive/developmental effects at doses which caused moderate dermal irritation. IOA is not genotoxic in vitro and did not cause an increased incidence of cancers in a limited dermal carcinogenicity study in mice.

Ecotoxicity: IOA is moderately to highly toxic to fathead minnows, daphnia, algae and bacteria. Bioconcentration is unlikely due to its rapid biodegradation and, by analogy to other acrylate esters, its rapid hydrolysis in vivo.

INITIAL ASSESSMENT

The potential for human exposure to IOA is very limited and its toxicity is low. Based on its use and hazard profile, the only anticipated human health risks posed by IOA are possible eye and skin irritation and allergic contact dermatitis among workers involved in its production or use. These effects are mitigated by the use of gloves by workers who may come into contact with the material.

IOA is manufactured in the U.S. by a single company as an intermediate for the synthesis of acrylic polymers. About 1000kg/year of IOA monomer is sold as a component of a concrete sealing product which is polymerized at the job site. Waste monomer is incinerated. There is no intentional discharge of IOA to water. Although IOA is significantly toxic to aquatic organisms and bacteria it is readily biodegraded. Airborne IOA concentrations in emissions from processing operations are typically less than 1ppm. Small quantities of unreacted IOA monomer are expected to reach landfills as a trace residual contaminant of certain industrial and consumer products. Atmospheric oxidation of IOA is expected to be rapid. There are no known or anticipated exposures to terrestrial organisms.

CONCLUSIONS AND RECOMMENDATIONS

Based on its low occupational exposure potential, its low toxicity in vitro and mammalian studies, its limited release to the environment

and its predicted rapid environmental biodegradation, IOA is considered a low priority for additional human health or environmental effects testing at this time.

Production - Trade

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Geographic Area : USA

General Comments : No non-confidential data available. The 3M company, St Paul, MN is believed to be the only manufacturer of IOA.

References

!SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Uses

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Geographic Area : USA

Use

Quantity	Year	Comments.
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>99%		An intermediate for the synthesis of acrylic polymers.
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1000 kg		A single product containing unreacted IOA as an intentional component is sold by 3M company as a concrete sealer for use by professional tradespeople.
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IOA in this product is
polymerized on the job site.

<0.1% Trace amounts of unreacted
IOA monomer are present in a
number of industrial and
consumer products (e.g.
adhesive tapes sold by 3M
company).

References

Secondary References : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, (1993)

Study

End Point : Pathway into the Environment and
Environmental Fate.

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Test Method and Conditions

Test method description : Method of Hunter, R., Faulkner, L,
Culver, F., and Hill, J., 1985, QSAR,
structure-activity based chemical
modelling and information software.
(Montana State University, Montana,
U.S.A.)

Quantity Transported

Medium to Medium Quantity Time Year to Year

to AIR <1.0 mg/l

For expected worst case operations. (Reported as <1.0ppm, which is
the detection limit).

to AQ FRESH

No intentional discharge to water.

to SOIL WASTE

Unspecified small amounts of unreacted IOA monomer are expected to reach landfills as a trace residual contaminant of certain industrial and consumer products.

to AIR 9.77%

According to "Neely 100-day partitioning pattern" (QSAR)

to AQ 50.83%

According to "Neely 100-day partitioning pattern" (QSAR)

to SOIL GRND 20-38%

According to "Neely 100-day partitioning pattern" (QSAR)

to SED 19.02%

According to "Neely 100-day partitioning pattern" (QSAR)

References

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point : HUMAN INTAKE AND EXPOSURE

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Evaluations

Evaluation text : 3M is believed to be the only

manufacturer of IOA. It is estimated that approximately 200 3M employees work in areas in which exposure to IOA, either as the liquid or vapor, could occur. Certain processes involving IOA are open systems in which IOA vapor may be generated. Ventilation systems are used to keep IOA vapor concentrations below the 3M Exposure Guideline of 5ppm (8h TWA). Air monitoring studies of 3M processing and manufacturing areas have typically indicated airborne IOA concentrations to be less than 1 ppm. Impermeable gloves are required to be worn by all employees who may come into contact with unreacted IOA monomer.

References

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point : BIODEGRADATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Geographic Area : USA

Test Subject

Organism Medium Specification

AQ

Test Substance

Impurities : Methyl ethyl hydroquinone 10-15ppm

Test Method and Conditions

Test method description : OECD Guideline 301d. Closed system.

(An)aerobic : AEROB

Exposure

Exposure Period : 5-28 d

Test Results

Quantity	Time	Comments on result
72%	AV	5 d In the uninhibited samples. Dissolved oxygen levels declined in proportion to test substance levels.
100%	AV	15-28 d In the uninhibited samples. Dissolved oxygen levels declined in proportion to test substance levels.
0.4%	AV	5 d In the inhibited samples with no oxygen depletion.
30%	AV	15 d In the inhibited samples with no oxygen depletion.
6.9%	AV	28 d In the inhibited samples with no oxygen depletion

The sodium benzoate reference solution showed dissolved oxygen loss of 56, 74 and 83% at 5, 15, 28 days, respectively.

General Comments : Biodegradation results indicate that IOA (the test substance) is treatable in sewage systems.

References

Primary Reference : #UR3MD*

Unpublished 3M Data

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, (1993)

Study

End Point : BIODEGRADATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Evaluations

Evaluation text : Information on treatability of the
substance: biodegradation results
indicate IOA is treatable in sewage
systems,

References

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, (1993)

Study

End Point : PHOTODEGRADATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Test Method and Conditions

Test method description : Estimate by the method of William Meylan
and Philip Howard, 1990. Atmospheric
oxidation program, version 1.10,
Syracuse Research Corporation, Syracuse,
N.Y., U.S.A.

Test Results

Quantity	Time	Comments on result
50%	6,5 d	Half life due to reaction with ozone at an ozone concentration of $7 \times E+11$ mol/cm ³ .

References

Primary Reference : #UR3MD*

Unpublished 3M Data

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point : HYDROLYSIS

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Test Method and Conditions

Test method description : Estimated by the method of William Meylan and Philip Howard, 1990. Atmospheric oxidation Program, version 1.10. Syracuse Research Corporation, Syracuse, N.Y. U.S.A.

Test Results

Quantity	Time	Comments on result
50%	11 h	T/2 due to reaction with hydroxyl radical at a hydroxyl radical concentration of $5 \times E+5$ mol/cm ³ .

(Half-life reported as 0.46 day).

References

Primary Reference : UR3MD*

Unpublished 3M Data

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, (1993)

Study

End Point : BIOCONCENTRATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Evaluations

Evaluation text : Bioaccumulation is not anticipated since
IOA is biodegradable and similar
acrylate esters are readily metabolized
in vivo.

References

Secondary Reference : !SIDSP*

OECD/SIDS, Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, (1993)

Study

End Point : MAMMALIAN ACUTE TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Species/strain/system : Sprague-Dawley strain

Dose / Concentration : 5000 mg/kg BW

Test Method and Conditions

Test method descriptions : 5 male and female rats were fasted overnight and administered undiluted substance monomer at a dose of 5g/kg body weight by oral gavage. OECD 401; GLP: YES

Test Results

Organism Medium Spec. Route Lifestage Sex Effect Effect Comments

RAT	ORL	ADULT	LD50	Rat oral LD50 was greater than 5g/kg body weight under the condition of the study.
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General Comments : Test results: no treatment-related mortality occurred during the study. Average body weights for male and female rats increased 43% and 13%, respectively, over the course of the study. Clinical signs consistent with gastrointestinal irritation (diarrhea) and mild central nervous system depression (ataxia and hypoactivity) were observed in most of the animals for the first two days after dosing. No significant gross lesions were noted at necropsy.

References

Primary Reference : JTEHD6

Gordon, S.C. et al. Journal of Toxicology and Environmental Health, 34, 279-296, (1991)

Secondary Reference : !SIDSP*

OECD/SIDS, Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, (1993)

Study

End Point : MAMMALIAN TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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RAT		SKN		ADULT			
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Species/strain/system : F344 rats strain

Test Substance

Vehicle - Solvent : Acetone

Test Method and Conditions

Test method description : OECD Combined Repeated Dose and
Reproductive/Developmental Screening
Test.

Exposure

Exposure Type : SHORT

Dose / Concentration : 1-25%

Exposure comments : Dermal application of 0%, 1%, 7.5%, 15%
or 25% of the substance solution in
acetone at a constant dose volume of
100ul/day. Due to marked irritation at

the treatment site in the high dose group the concentration was lowered to 20% after one week.

Test Results

Organ	Effect	Rev.	OnSet	Affected in Sex	Exposed - Controls
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SKIN	IRRIT			M	
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CIRC

STRUC

Dermal irritation was observed in the high dose group and included slight to moderate erythema and slight desquamation.

SKIN	IRRIT			F	
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CIRC

STRUC

Dermal irritation was observed in the high dose group and included slight erythema, slight to moderate desquamation and slight fissuring.

BLOOD	BIOCH			M	
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Minimally higher serum aspartate and alanine aminotransferases levels were observed in the high dose group.

General Comments : There were no significant differences (as compared with controls) in body weights, absolute organ weights, organ to body weights percentages, or macroscopic and microscopic findings for any dose group.

References

Primary Reference : #UR3MD*

Unpublished 3M Data, (1992)

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, 12, (1993)

Study

End Point : CARCINOGENICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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MOUSE		SKN	74-79 d	M		40/GROUP	
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Species/strain/system : C3H/HeJ mice strain

Test Substance

Vehicle - Solvent : Acetone

Test Method and Conditions

Test method description : EPA recommendations for dermal screening
for carcinogenesis of
acrylates/methylacrylates. GLP: NO.

Exposure

Exposure Type : LONG

Frequency : 3 x/wk

Dose/Concentration : 5 % v/v

Exposure comments : Carcinogenicity potential was studied in
a lifetime dermal bioassay. 25ul of the

substance monomer or acetone (negative solvent control) were applied to shaved backs of the animals three days/week. Daily observation for mortality and monthly examination for skin lesions were done. Necropsy was performed on all animals.

Test Results

Organ	Effect	Rev.	OnSet	Affected in Sex	Exposed - Controls
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SKIN	CIRC			M	
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CHNG

Gross and microscopic dermal lesions observed in the IOA-treatment group were: edema (1/39 animals), surface crusting (10/39), epidermal vesiculation (1/39), hyperkeratosis (27/39).

SKIN	STRUC				
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NEO

Epidermal hyperplasia (16/39) and benign melanoma (1/39) were reported.

NEF

No significant difference in mean survival time between treatment and control groups.

General Comments : Microscopic examination of the melanoma showed that the cells were well differentiated with no indication of nuclear or cytoplasmic pleomorphism or atypia. Study performed at Bushy Run Research Center, Export, PA in April 1979.

References

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, 16-17,
(1993)

Study

End Point : MUTAGENICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number
controls

BACT VTR

Species/strain/system : Salmonella typhimurium strains: TA98,
TA100, TA1535, TA1537 and TA1538.

Test Substance

Vehicle - Solvent : Dimethylsulfoxide (DMSO)

Test Method and Conditions

Test method descriptions : Essentially similar to OECD 471; GLP: NO

Exposure

Exposure Type : SHORT

Dose / Concentration : 0.005-0.5 ul/ PLATE

Exposure comments : Ames salmonella microsome assay with and
without metabolic activation was
performed in quadruplicate with 6
concentrations. Negative controls were

run with DMSO and positive controls with
2-anthramine, sodium azide,
9-aminoacridine or 2-nitrofluorene.

Test Results

Organ	Effect	Rev.	OnSet	Affected in Sex	Exposed - Controls
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CELL

The highest concentration tested: 0.5ul/plate, produced pinpoint colonies, (indication of toxicity), in strain TA100.

NEF

No significant increase in revertants were observed at any IOA concentration, either with or without metabolic activation.

General Comments : IOA was not considered mutagenic under the conditions of the study.

References

Primary Reference : JTEHD6

Gordon, S.C. et al. Journal of
Toxicology and Environmental Health, 34,
297-308, (1991)

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, 12, (1993)

Study

End Point : MUTAGENICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

FUNGT VTR

Species/strain/system : Saccharomyces cerevisiae D3 strain

Test Substance

Vehicle - Solvent : DMSO

Test Method and Conditions

Test method descriptions : Testing for mitotic recombinogenic activity following the method of Zimmerman and Schwater. GLP: NO

Exposure

Exposure Type : SHORT

Dose / Concentration : 0.00005.0.05 % v/v

Exposure comments : Test with and without metabolic activation was run at seven concentrations of IOA, DMSO was used for negative control and 1,2,3,4-diepoxybutane for the positive control.

Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in Exposed - Controls
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CELL

Toxic effect was observed at concentration of 0.05% with metabolic activation and at 0.01% without metabolic activation.

NEF

IOA was not mutagenic under the test conditions.

General Comments : Study performed at SRI international,
Menlo Park, CA, in May 1980.

References

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, 13-14,
(1993)

Study

End Point : MUTAGENICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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MOUSE			VTR				
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Species/strain/system : Mouse embryo C3H/10T1/2 cell line

Test Substance

Vehicle - Solvent : Acetone

Test Method and Conditions

Test method description : Cell transformation potential according
to Bertram; GLP: YES. Transformation was

classified according to the criteria of
Reznikoff.

Exposure

Dose / Concentration : 0.0049-0.039 ul/ml

Exposure comments : Four concentrations, 12
plates/concentration. Acetone was used
for the negative control tests and 7,12-
dimethylbenz(a)anthracene for the
positive control. (Cancer Res. 33, 3231,
1973)

Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in Exposed - Controls
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NEF

No type II or type III transformed foci were observed in any of the
IOA cultures.

CELL

Lowest concentration producing cell toxicity was 0.0098ul/ml, without
metabolic activation.

General Comments : IOA did not cause morphological
transformation of C3H/10T1/2 cells in
this test system.

References

Primary Reference : CNREA8

Bertram. Cancer Research, 37, 514,
(1977)

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, 14, (1993)

Study

End Point : MUTAGENICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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MOUSE			VTR				
-------	--	--	-----	--	--	--	--

Species/strain/system : Mouse lymphoma, L5178Y TK +/- cells

Test Substance

Vehicle - Solvent : Dimethylsulfoxide

Test Method and Conditions

Test method descriptions : According to a modification of the method of Clive and OECD 476. GLP: YES

Exposure

Dose / Concentration : 0.0015-0.11 ul/ml

Exposure comments : Mutagenic activity assay was performed with and without metabolic activation at concentrations 0.0084-0.11 ul/ml and 0.0015-0.02 respectively, (In triplicates). DMSO was used in the negative control. Ethylmethanesulfonate and 7,12-dimethylbenz(a)anthracene were used in the positive control.

Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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PHENO CHNG

One concentration without metabolic activation and three concentrations with metabolic activation had mutant frequencies which were two-fold greater than the solvent control. Dose related increases were not observed.

CELL

Lowest concentration producing cell toxicity was 0.063ul/ml, without metabolic activation was 0.0036ul/ml. IOA was not considered mutagenic under the conditions of the assay.

References

Primary Reference : MUREAV

Clive, D. and Spencer, J. F. S. Mutation
Research, 31, 17, (1975)

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, 15, (1993)

Study

End Point : IRRITATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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RBT

SKN

Species/strain/system : New Zealand rabbits strain

Test Method and Conditions

Test method description : U.S. Federal Hazardous Substances Act
test guidelines. 0.5ml undiluted samples
to both abraded and intact skin. GLP:
NO.

Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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SKIN CIRC

Slight erythema (no edema) was noted at each test site in all of the
test animals at both the 1 and 48 hour examination.

SKIN IRRIT

The mean primary dermal irritation score was 1.0 at both examination
times.

General Comments : Conclusions: IOA was slightly irritating
under the conditions of the study.

References

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, 11, (1993)

Study

End Point : IRRITATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

RBT OCU ADULT

Species/strain/system : New Zealand rabbits

Test Method and Conditions

Test method description : U.S. Federal Hazardous Substances Act
test guidelines. GLP: NO.

Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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EYE IRRIT

At the 1 hour examination all animals showed slight discharge from the treated eye and 4/6 had slight conjunctival swelling. No evidence of irritation was noted at any other examination time up to 7 days.

General Comments : IOA monomer was slightly irritating
under the conditions of the study.

References

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, 11, (1993)

Study

End Point : REPRODUCTION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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RAT			SKN				
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Species/strain/system : F344 rats

Test Substance

Vehicle - Solvent : Acetone

Test Method and Conditions

Test method description : OECD Combined Repeated Dose and Reproductive/Developmental Screening test. GLP: YES.

Exposure

Exposure Type : SHORT

Dose / Concentration : 1-25%

Exposure comments : Dermal application of 0%, 1%, 7.5%, 15% or 25% of IOA solution in acetone at a volume dose of 100ul/day. Due to marked irritation at the treatment site in the high dose group, the concentration was lowered to 2% after one week.

Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in Exposed - Controls
-------	--------	------	-------	-----	--------------------------------

NEF

F

No overt maternal toxicity was noted at any dose level tested. The no-observable-effect-level NOEL for reproductive and developmental testing was 20%* IOA.

General Comments : *Severe dermal irritation at infusion site precluded dosing at higher concentrations. For other dermal effects see the results of repeated dose toxicity testing

References

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 17, (1993)

Study

End Point : AQUATIC ACUTE TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Species/strain/system : Fathead minnows juvenile (Pimephales promelas) mean length=1.6cm

Exposure Period : 96 h

Test Method and Conditions

Test method description : OECD Guideline 203

Test Results

Organism Medium Spec. Route Lifestage Sex Effect Effect Comments

FISH AQ FRESH LC50 Lethal concentration LC50 = 0.67mg/l for 96h. NOEC (no observed effect concentration) = 0.34mg/l.

General Comments : Results based on mean measured concentration.

References

Secondary Reference : ISIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point : AQUATIC TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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BACT	AQ	MARIN					
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Species/strain/system : Bacteria bioluminiscent (Photobacterium phosphorium)

Test Substance

Description of the test : Test substance: lot 1419 substance

Test Method and Conditions

Test method description : Microtox(R) Toxicity Analyser, Model 2055 (Microbics Corp.) which measures the reduction in bioluminescence of naturally occurring marine bacterium in response to chemical toxicant.

Exposure

Exposure Period : 5-15 mi

Dose / Concentration : 0.034-0.27 mg/l

Exposure comments : Two separate tests were run with four concentrations of test substance, ranging from 0.034-0.27mg/l.

Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in Exposed - Controls
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CHNG

Inhibitory concentration IC50 for reduction in bioluminescence = 0.163mg/l for 5 minutes and 0.168mg/l for 15 minutes.

References

Primary Reference : #UR3MD*

Unpublished 3M Data

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point : AQUATIC TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number
controls

CRUS AQ FRESH

Species/strain/system : Water flea (*Daphnia magna*), less than
24h old neonates

Test Substance

Description of the test : Test substance: lot 1419
substance

Test Method and Conditions

Test method description : OECD Guideline 202. GLP specified.
Immobilization test.

Exposure

Exposure Type : ACUTE

Exposure Period : 48 h

Dose/Concentration : <0.24-0.77 mg/l

Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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BEHAV

EC50

Effective Concentration for immobilization, EC50 = 0.77mg/l for 48h
(test result based on initial measured concentrations).

EC50 = 0.40mg/l for 48h (test result based on mean measured
concentrations).

BEHAV

NOEC

No Observed Effect Concentration NOEC = $\lt; 0.56\text{mg/l}$ (test result based on initial measured concentrations). NOEC = $\lt; 0.24\text{mg/l}$ for 48h. (Test result based on mean measured concentrations).

References

Primary Reference : #UR3MD*

Unpublished 3M Data

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point : AQUATIC TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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CRUS	AQ	FRESH					
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Species/strain/system : Water flea (Daphnia magna), less than 24h old neonates

Test Substance

Description of the test : Test substance: lot 3290 substance

Test Method and Conditions

Test method description : OECD Guideline 202. GLP specified.

Exposure

Exposure Type : LONG

Exposure Period : 14-21 d

Dose / Concentration : <0.13 -2.93 mg/l

Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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EC50

Effective Concentration, EC50 = 2.93mg/l for 14 days, EC50 = 2.62mg/l for 21 days. (Test results based on initial measured concentrations).

Inhibitory concentration IC50 = 1.50mg/l for 14 days. IC50 = 1.72mg/l for 21 days. (Test results based on initial measured concentrations).

NOEC

No Observed Effect Concentration NOEC = 0.79mg/l for 14 days. NOEC = <0.20 mg/l for 21 days, (Test result based on initial measured concentrations).

EC50

EC50 = 1.99mg/l for 14 days. EC50 = 1.61mg/l for 21 days. (Test result based on mean measured concentrations).

IC50 = 0.97mg/l for 14 days. IC50 = 1.02mg/l for 21 days. (Test result based on mean measured concentrations).

NOEC

NOEC = 0.51mg/l for 14 days. NOEC = <0.13 mg/l for 21 days. (Test result based on mean measured concentrations).

References

Primary Reference : #UR3MD*

Unpublished 3M Data

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data
Set (SIDS) of OECD High Production
Volume Chemicals Programme, (1993)

Study

End Point : AQUATIC TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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FISH	AQ	FRESH					
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Species/strain/system : Fathead minnows juvenile (Pimephales
promelas) mean length=1.6cm

Test Method and Conditions

Test method description : OECD Guideline 203

Exposure

Exposure Period : 96 h

Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in	Exposed - Controls
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NOEC

No Observed Effect Concentration, NOEC = 0.34mg/l for 96h

General Comments : Test result based on mean measured concentrations.

References

Secondary Reference : !SIDSP*

OECD/SIDS Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Substance

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Description

Option for disposal: all waste IOA monomer generated by 3M is incinerated in a hazardous waste incinerator. There is no intentional discharge to water. It is anticipated that consumer and industrial products containing trace amounts of unreacted IOA monomer (typically less than 0.1% by weight) may be landfilled or incinerated after their use.

References

Secondary Reference : !SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)