I U C L I D

D a t a s e t

Existing Chemical	Substance ID: 110–19–0
CAS No.	110–19–0
EINECS Name	isobutyl acetate
EINECS No.	203–745–1
Molecular Formula	C6H12O2

Dataset created by: EUROPEAN COMMISSION – European Chemicals Bureau

This dossier is a compilation based on data reported by the European Chemicals Industry following 'Council Regulation (EEC) No. 793/93 on the Evaluation and Control of the Risks of Existing Substances'. All (non–confidential) information from the single datasets, submitted in the IUCLID/HEDSET format by individual companies, was integrated to create this document.

The data have not undergone any evaluation by the European Commission.

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1.0.1 OECD and Company Information

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Country: Italy
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Name: BASF AG
Street: Karl–Bosch–Str
Town: 67056 Ludwigshafen
Country: Germany

Name: BASF Espanola S. A.
Town: 43080 Tarragona
Country: Spain

Name: BP Chemicals Ltd.
Street: 76, Buckingham Palace Road
Town: SW1 WOSU London
Country: United Kingdom

Name: BRENNTAG International Chemicals GmbH
Street: Humboldtring 15
Town: 45472 Mülheim
Country: Germany
Phone: 0208/494431
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Name: Eastman Chemical (Deutschland) GmbH
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Town: D–51149 Koln
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Telex: 887012

Name: Enichem S.p.A.
Street: Via Taramelli,26
Town: 20124 Milan
Country: Italy

Name: Huels AG
Street: Postfach
Town: D–45764 Marl
Country: Germany

Name: NEUBER GES.M.B.H.
Street: BRÜCKENGASSE 1
Town: 1060 WIEN
Country: Austria
Phone: 0222/599950
Telefax: 0222/5970200

Name: Rohm and Haas France S.A.
Street: 371 rue L. van Beethoven
Town: 06565 Valbonne
Country: France

Name: Union Carbide Benelux
Street: Norderlaan 147
Town: 2030 Antwerpen
Country: Belgium

1.0.2 Location of Production Site

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1.0.3 Identity of Recipients

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1.1 General Substance Information

Substance type: organic
Physical status: liquid

1.1.1 Spectra

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1.2 Synonyms

.beta.–Methylpropyl ethanoate
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

2–Methyl–1–propyl acetate
Source: Huels AG Marl

2–Methylpropyl acetate
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Eastman Chemical (Deutschland) GmbH Koln

2–Methylpropyl acetate
Source: Huels AG Marl

(1)

ACETATO DI ISOBUTILE
Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

acetic acid isobutyl ester
Source: Union Carbide Benelux Antwerpen

acetic acid, 2–methylpropyl ester
Source: Union Carbide Benelux Antwerpen

Acetic acid, 2–methylpropyl ester
Source: Huels AG Marl
Eastman Chemical (Deutschland) GmbH Koln

Acetic acid, 2–methylpropyl ester (9CI)
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

Acetic acid, isobutyl ester
Source: Eastman Chemical (Deutschland) GmbH Koln

Acetic acid, isobutyl ester (6CI, 8CI)
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

Acetic acid, isobutylester
Source: Huels AG Marl

beta–methylpropyl ethanoate
Source: Union Carbide Benelux Antwerpen

beta–Methylpropyl ethanoate
Source: Huels AG Marl

beta–methylpropylethanoate; 2–methyl–1–acetate; isobutyl acetate; Acetato di isobutile (Italian)
Source: Enichem S.p.A. Milan

Essigsaeure–isobutylester
Source: Huels AG Marl

Essigsäure–i–butylester
Source: BRENNTAG International Chemicals GmbH Mülheim

ISOBUTILACETATO
Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

Isobutyl acetate
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Huels AG Marl

Isobutyl ethanoate
Source: Eastman Chemical (Deutschland) GmbH Koln

1.3 Impurities

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1.4 Additives

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1.5 Quantity

Quantity 100 000 – 500 000 tonnes

1.6.1 Labelling

Labelling: as in Directive 67/548/EEC
Symbols: F
Nota: C
D
Specific limits: no data
R–Phrases: 1
S–Phrases: (2) Keep out of reach of children
(16) Keep away from sources of ignition – No smoking
(23) Do not breathe ...
(25) Avoid contact with eyes
(29) Do not empty into drains
(33) Take precautionary measures against static discharges

1.6.2 Classification

Classification: as in Directive 67/548/EEC
Class of danger: highly flammable
R–Phrases: (11) Highly flammable

Classification: as in Directive 67/548/EEC
Class of danger:
R–Phrases: 6

1.7 Use Pattern

Type: type
Category: Non dispersive use

Type: type
Category: Use in closed system

Type: type
Category: Wide dispersive use

Type: industrial
Category: Basic industry: basic chemicals

Type: industrial
Category: Paints, lacquers and varnishes industry

Type: industrial
Category: Polymers industry

Type: industrial
Category: other: industrial ink

Type: industrial
Category: other: resins

Type: industrial
Category: other

Type: use
Category: Adhesive, binding agents

Type: use
Category: Solvents

1.7.1 Technology Production/Use

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1.8 Occupational Exposure Limit Values

Type of limit: MAK (DE)
Limit value: 200 ml/m3
Short term expos.
Limit value: 400 ml/m3
Schedule: 5 minute(s)
Frequency: 8 times
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

(2)

Type of limit: MAK (DE)
Limit value: 950 mg/m3
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

(2)

Type of limit: MAK (DE)
Limit value: 950 mg/m3
Short term expos.
Limit value: 950 mg/m3
Country: Germany
Source: Huels AG Marl

Type of limit: MAK (DE)
Limit value: 200 ml/m3
Short term expos.
Limit value: 200 ml/m3
Country: Germany
Source: Huels AG Marl

Type of limit: OES (UK)
Limit value: 150 ml/m3
Short term expos.
Limit value: 187 ml/m3
Source: BP Chemicals Ltd. London

Type of limit: OES (UK)
Limit value: 713 mg/m3
Source: Eastman Chemical (Deutschland) GmbH Koln

Type of limit: TLV (US)
Limit value: 713 mg/m3
Source: Union Carbide Benelux Antwerpen

(3)

Type of limit: TLV (US)
Limit value: 713 mg/m3
Source: Enichem S.p.A. Milan

(4)

Type of limit: TLV (US)
Limit value: 713 mg/m3
Short term expos.
Limit value: 888 mg/m3
Schedule: 15 minute(s)
Frequency: 4 times
Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

Type of limit: TLV (US)
Limit value: 713 mg/m3
Source: Eastman Chemical (Deutschland) GmbH Koln

Type of limit: other: MAK (Österreich)
Limit value: 700 mg/m3
Source: NEUBER GES.M.B.H. WIEN

Type of limit: other: twa
Limit value: 150 other: ppm
Short term expos.
Limit value: 187 other: ppm
Source: Rohm and Haas France S.A. Valbonne

1.9 Source of Exposure

Memo: Emissionserklaerung Huels 1992
Remark: Release into the atmosphere on production site in 1992: 1000 kg/a
Source: Huels AG Marl

(5)

Remark: As the quantities of this substance placed on the EU market by Union Carbide Benelux N.V. are normally sourced from the manufactruing facilities of its U.S. parent company, no exposure can arise within the EU from the manufacture of these quantities. The comments below on exposure are restricted to uses for which Union Carbide believes its customers use this substance.

Major use(s): As paint solvent.

Sources of human exposure: In industrial applications, negligible human exposure assuming appropriate industrial hygiene and personal protective precautions are observed. Consumer applications may result in minor exposure by inhalation and/or skin contact. No quantitative estimates are available.

Sources of environmental exposure: Releases to the atmosphere from industrial installations not equipped with incinerators, and from professional and public users of paint formulations containing this substance. Releases to the water compartment by professional and public users will occur. The substance is readily biodegraded in waste water treatment systems. No quantitative estimates of releases are available.
Source: Union Carbide Benelux Antwerpen

Remark: Substance not imported into EU as such but only as solvant in preparations.
Source: Rohm and Haas France S.A. Valbonne

Remark: La sostanza in esame è prodotta nello stabilimento Distillerie Italiane dell'Alusuisse Italia Spa.
Il processo è di tipo continuo e consiste essenzialmente nelle seguenti fasi:

- Reazione
- Lavaggio
- Purificazione

Le fasi del processo vengono condotte a ciclo chiuso in quanto tutte le sostanze coinvolte nella sintesi chimica sono movimentate attraverso pompe , tubazioni, sistemi di trasferimento e apparecchiature di tipo chiuso.
Gli effluenti del processo sono i seguenti:
1) Acqua di reazione
2) Gas incondensabili

L'acqua di reazione, contenente tracce di sostanze

organiche, viene raccolta e trasferita al trattamento di depurazione nell'impianto chimico biologico dello Stabilimento, quindi immessa in acque superficiali nei limiti stabiliti
dalle leggi nazionali (Legge Merli n° 319/76).

I gas ricondensabili, contenenti tracce di sostanze organiche, provenienti dalle apparecchiature di processo, prima dell'immisione in atmosfera,Vengono refrigerati in appositi scambiatori per il recupero dell'organico presente;

Dati relativi alle emissioni

Acque trattate :

* tipo di emissione – puntiforme
* Portata – 0,3 m3/h per Ton. di prodotto
* Durata emissione – continua

Fattori potenziali di esposizione umana

Nel processo di fabbricazione:
Considerato le caratteristiche dell'impianto di produzione (ciclo chiuso e processo di tipo continuo) si ritiene insignificante il potenziale di esposizione alla sostanza da parte dell'operatore.

Settori di impiego

La sostanza fa parte della famiglia dei solventi e viene impiegata nel settore delle vernici.

Processi relativi ai settori di impiego

La sostanza viene miscelata a temperatura ambiente agli altri componenti della vernice in apparecchiature di tipo chiuso; la vernice risultante viene caratterizzata e quindi confezionata in impianti dotati di aspirazioni localizzate.

Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

Source: Eastman Chemical (Deutschland) GmbH Koln

1.10.1 Recommendations/Precautionary Measures

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1.10.2 Emergency Measures

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1.11 Packaging

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1.12 Possib. of Rendering Subst. Harmless

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1.13 Statements Concerning Waste

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1.14.1 Water Pollution

Classified by: KBwS (DE)
Labelled by: KBwS (DE)
Class of danger: 1 (weakly water polluting)
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

Classified by: KBwS (DE)
Labelled by: KBwS (DE)
Class of danger: 1 (weakly water polluting)
Country: Germany
Remark: Katalog-Nr.: 133
Source: Huels AG Marl

(6)

1.14.2 Major Accident Hazards

Legislation: Stoerfallverordnung (DE)
Substance listed: yes
Remark: Stoerfall-Stoff-Nr.2 "leicht entzuendliche Fluessigkeiten"
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

(7)

Legislation: Stoerfallverordnung (DE)
Substance listed: yes
Country: Germany
Remark: in Anhang IV genannt (Kat.6; leichtentzuendliche Fluessigkeiten) Nr. 213
Source: Huels AG Marl

(8) (9)

1.14.3 Air Pollution

Classified by: TA-Luft (DE)
Labelled by: TA-Luft (DE)
Number: 3.1.7 (organic substances)
Class of danger: III
Source: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

Classified by: other: VCI
Labelled by: other: VCI
Number: 3.1.7 (organic substances)
Class of danger: III
Country: Germany
Source: Huels AG Marl

(8)

1.15 Additional Remarks

Remark: Disposal: Incinerate in a furnace where permitted under national and local regulations.

Transport: Isobutyl acetate is a class 3 product according the ADR/RID/IMDG/ICAO regulations.

This substance is shipped in road/rail tankcars, tankcontainers/ISOtanks and smaller packages (e.g. drums).
Source: Union Carbide Benelux Antwerpen

Remark: Possibilità di eliminazione

La sostanza ha una bassa solubilità in acqua; può essere eliminata per ossidazione biologica in appositi impianti di depurazione. Eventuali scarti/rifiuti contenenti la sostanza possono essere eliminati per ossidazione termica in impianti appositi di incenerimento con recupero energetico e controllo emissioni all'atmosfera secondo la normativa vigente (DPR 203/88)

Informazioni relative al trasporto

La sostanza, stoccata in serbatori fuori terra viene spedita alla rinfusa con autobotti.

Trasporto in strada Nazionale/Internazionale

- Tipo del mezzo: autobotte/autocisterna per prodotti ADR. classe 3 3°/b 33/1213

- Quantità media trasportata (autobotti/autocisterna) : 23.000 KG

- Automezzi/mese : 20-40

- Misure di controllo durante il trasporto : Il prodotto viaggia con la documentazione stabilita dalle leggi vigenti in materia di prodotti ADR.

Viene consegnata all'autista la scheda TREM CARD, con notizie utili al soccorso stradale, in caso di incidente.
Source: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

Remark: iso–Butyl acetate is shipped either in bulk or in steel drums. Bulk shipments are by tank trucks, rail tank cars, or rail tank containers. Our warehouses are checking that the transporters have the necessary papers and equipment for the shipment of a hazardous material.
Source: Eastman Chemical (Deutschland) GmbH Koln

1.16 Last Literature Search

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1.17 Reviews

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1.18 Listings e.g. Chemical Inventories

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2.1 Melting Point

Value: = -99.5 degree C
Method: other
GLP: no data
Source: Huels AG Marl
(10)

Value: = -99 degree C
Decomposition: no
Sublimation: no
Method: other: nicht bekannt
GLP: no data
Source: NEUBER GES.M.B.H. WIEN

Value: = -99 degree C
GLP: no
Source: Huels AG Marl
(11)

Value: = -70 degree C
Source: BASF AG Ludwigshafen
(12)

Value: = -70 degree C
Source: Huels AG Marl
(13)

2.2 Boiling Point

Value: = 111 - 118 degree C at 1013 hPa
Method: other: DIN 53 171
Source: BASF AG Ludwigshafen
(12)

Value: = 111 - 118 degree C at 1013 hPa
Method: other: DIN 53171
Source: Huels AG Marl
(13)

Value: = 112.5 degree C at 1013 hPa
GLP: no data
Source: Huels AG Marl
(10)

Value: 114 - 118 degree C at 1013 hPa
Decomposition: no
GLP: no
Source: Huels AG Marl
(11)

Value: = 115 - 118 degree C
Decomposition: no
Method: other: DIN 53171
GLP: no data
Source: NEUBER GES.M.B.H. WIEN

2.3 Density

Type: density
Value: = .858 g/cm3 at 20 degree C
Source: BASF AG Ludwigshafen
(12)

Type: density
Value: = .858 g/cm3 at 20 degree C
Source: Huels AG Marl
(13)

Type: density
Value: = .869 - .872 g/cm3 at 20 degree C
GLP: no
Source: Huels AG Marl
(11)

Type: density
Value: = .87 g/cm3 at 20 degree C
Method: other: DIN 51757
GLP: no data
Source: NEUBER GES.M.B.H. WIEN

Type: density
Value: = .87 g/cm3 at 20.5 degree C
GLP: no data
Source: Huels AG Marl
(10)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: = 18 hPa at 20 degree C
GLP: no
Source: Huels AG Marl
(11)

Value: = 19 hPa at 20 degree C
Method: other (measured): DIN 51754
GLP: no data
Source: NEUBER GES.M.B.H. WIEN

Value: = 500 hPa at 20 degree C
Source: BASF AG Ludwigshafen
(12)

Value: = 500 hPa at 20 degree C
Source: Huels AG Marl
(13)

Value: = 16.6 hPa at 20.5 degree C
GLP: no data
Source: Huels AG Marl
(10)

2.5 Partition Coefficient

log Pow: = 1.72
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year: 1981
GLP: no
Source: Huels AG Marl
(14)

2.6.1 Water Solubility

Value: = 6 g/l at 20 degree C
pH: 5 at 4 g/l and 20 degree C
Source: BASF AG Ludwigshafen
(12)

Value: = 6 g/l at 20 degree C
pH: 5 at 4 g/l and 20 degree C
Source: Huels AG Marl
(13)

Value: = 6.7 g/l at 20 degree C
GLP: no
Source: Huels AG Marl
(11)

Value: = 53 g/l at 20 degree C
Qualitative: of very low solubility
Source: NEUBER GES.M.B.H. WIEN

Value: = 7 g/l at 20.5 degree C
GLP: no data
Source: Huels AG Marl
(10)

2.6.2 Surface Tension

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2.7 Flash Point

Value: = 19 degree C
Type: closed cup
Method: other: DIN 51758
Year:
GLP: no data
Source: NEUBER GES.M.B.H. WIEN

Value: ca. 19 degree C
Type: closed cup
Method: other: DIN 51755
Year:
GLP: no
Source: Huels AG Marl
(11)

Value: = 21.5 degree C
Type: closed cup
Method:
Year:
GLP: no data
Source: Huels AG Marl
(10)

2.8 Auto Flammability

Value: = 385 degree C
Method: other: DIN 51 794
Source: BASF AG Ludwigshafen
(12)

Value: = 385 degree C
Method: other: DIN 51794
Source: Huels AG Marl
(13)

Value: = 427.5 degree C
Method: other: ASTM D 2155
GLP: no data
Source: Huels AG Marl
(10)

Value: = 480 degree C
Method: other: DIN 51794
GLP: no
Source: Huels AG Marl
(11)

2.9 Flammability

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2.10 Explosive Properties

Result: other
Remark: Explosive limits in air: 4.0 – 13.8 % (v/v)
Source: Huels AG Marl
(13)

Result: other
Remark: Explosive limits in air: 1.27 – 7.5 % (v/v)
Source: Huels AG Marl
(10)

Result: other
Remark: Explosive limits in air: 1.6 – 10.5 % (v/v)
Source: Huels AG Marl
(11)

Result:
Remark: Explosionsgrenzen in Luft: 4,0–13,8 Vol.%
Source: BASF AG Ludwigshafen
(12)

2.11 Oxidizing Properties

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2.12 Additional Remarks

Remark: viscosity (20 degree C): 0.69 mPa x s
pH–value (20 degree C): neutral
Source: Huels AG Marl
(11)

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 500000 molecule/cm3
Rate constant: = .0000000000055 cm3/(molecule * sec)
Degradation: = 50 % after 2.9 day
Method: other (measured): AOP Computer Program, Vers. 1.53, Syracuse Research Center (based on Reference)
Year: 1994 **GLP:**
Test substance:
Remark: half–life refers to 24 hour–days
Source: Huels AG Marl

(15)

3.1.2 Stability in Water

Type: abiotic
Method:
Year: **GLP:**
Test substance:
Result: The volatilization half–life from a river one meter deep flowing 1 m/s with a wind velocity of 3 m/s has been estimated to be 5.3 hours; the volatilization half–life from a similar river 10 m deep has been estimated to be 7.1 days. The hydrolysis half–lives of isobutyl acetate are probably similar to the half–lives of sec–butyl acetate which are about 12.6 years, 1.26 years, and 46 days at pHs 7.0, 8.0, and 9.0, respectively at 25 degree C.; this indicates that hydrolysis will be important only in very alkaline environmental waters. Aquatic adsorption to sediments and bioconcentration are not expected to be significant.
Source: HSDB print–out obtained from BP Chemicals
Huels AG Marl

(16)

3.1.3 Stability in Soil

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3.2 Monitoring Data (Environment)

Type of measurement: background concentration
Medium: air
Remark: Concentration in forest air (Kaelbelescheuer, Haldenhof, Rehauer; Black Forest, Germany): 2 – 218 ng/m3; Concentration in suburban air (Tuebingen): 38 – 284 ng/m3; samples were taken from March to October (year of examination not given).
Source: Huels AG Marl
Test condition: Tenax cartridges

(17)

3.3.1 Transport between Environmental Compartments

Type: adsorption
Media: water – soil
Method: other: Calculation from regression equation
Year:
Result: Based on log Kow of 1.60 and a water solubility of 6300 ppm at 25 degree C, the Koc value for isobutyl acetate can be estimated to be 177 and 36, respectively, by regression derived equations. These Koc values indicate a high to medium mobility.
Source: HSDB print–out obtained from BP Chemicals Huels AG Marl

(16)

3.3.2 Distribution

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

Air:	91.584 %
Soil:	0.037 %
Water:	8.345 %
Sediment:	0.034 %
Biota:	0.000 %

Source: Huels AG, Marl
Huels AG Marl
Test condition: Data used:

Molar mass:	116.16 g/mol
Log Pow:	1.72
Vapor pressure:	1800 Pa
Water solubility:	6.7 g/l

Equations used for additional data:
log Koc = 0.989 log Pow – 0.346

Volumes used:

Air:	6 000 000 000
Soil:	45 000
Water:	7 000 000
Sediment:	35 + 21 000
Biota:	7

3.4 Mode of Degradation in Actual Use

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3.5 Biodegradation

Type: aerobic
Inoculum: predominantly domestic sewage
Concentration: 10 mg/l related to DOC (Dissolved Organic Carbon)
Degradation: = 98 % after 21 day
Result: readily biodegradable
Method: OECD Guide-line 301 E "Ready biodegradability: Modified OECD Screening Test"
Year: 1981 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Source: Huels AG Marl

(14)

Type: aerobic
Inoculum: other: domestic sewage, non-adapted
Degradation: = 81 % after 20
Kinetic:

5	= 60 %
10	= 74 %
15	= 79 %

Method: other: Standard Method for the Examination of Water and Wastewater, APHA
Year: 1971 **GLP:** no data
Test substance: no data
Remark: test substance concentration 3 - 10 mg/l; biodegradation related to theoretical oxygen demand (ThOD)
Source: Huels AG Marl

(18)

Type: aerobic
Inoculum: other: seawater microorganisms, non-adapted
Degradation: = 37 % after 20
Kinetic:

5	= 23 %
10	= 35 %
15	= 37 %

Method: other: Standard Method for the Examination of Water and Wastewater, APHA
Year: 1971 **GLP:** no data
Test substance: no data
Remark: test substance concentration 3 - 10 mg/l; biodegradation related to theoretical oxygen demand (ThOD)
Source: Huels AG Marl

(18)

3.6 BOD5, COD or BOD5/COD Ratio

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3.7 Bioaccumulation

Species: other
Exposure period:
Concentration:
BCF:
Elimination:
Method:
Year: **GLP:**
Test substance:
Remark: Based on log Kow of 1.60 and a water solubility of 6300 ppm at 25 degree C, the BCF value for isobutyl acetate can be estimated to be 9.7 and 4, respectively, by regression derived equations. These BCF values suggest that bioconcentration is not significant.
Source: HSDB print–out obtained from BP Chemicals Huels AG Marl

(16)

3.8 Additional Remarks

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AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: flow through
Species: Leuciscus idus melanotus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC0: = 70 – 88
LC50: = 101 – 123
LC100: = 123 – 176
Method: other: DIN 384 12 L-20
Year: 1978 **GLP:** no data
Test substance: no data
Source: NEUBER GES.M.B.H. WIEN

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC50: = 190
Method: other: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Fische, DIN 38412 Teil 15
Year: 1982 **GLP:** no
Test substance: as prescribed by 1.1 – 1.4
Source: Huels AG Marl

(14)

Type: static
Species: Leuciscus idus melanotus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC0: = 70
LC50: = 101
LC100: = 123
Method: other: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Fische, DIN 38412 Teil 15; Vorabdruck 1976
Year: 1976 **GLP:** no data
Test substance: no data
Source: Huels AG Marl

(19)

Type: static
Species: Leuciscus idus melanotus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC0: = 88
LC50: = 123
LC100: = 176
Method: other: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Fische, DIN 38412 Teil 15; Vorabdruck 1976
Year: 1976 **GLP:** no data
Test substance: no data
Source: Huels AG Marl

(19)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Artemia salina (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: = 1200
Method: other: Acute Toxicity Test
Year: 1974 **GLP:** no data
Test substance: no data
Source: Huels AG Marl
Test condition: 24.5 degree C

(18)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = 168
Method: other: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Kleinkrebse, Daphnien-Kurzzeittest, DIN 38412 Teil 11
Year: 1982 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: 95 % confidence interval: 146.8 to 192.2 mg/l
Source: Huels AG Marl

(20)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC0: = 39
EC50: = 250
EC100: = 1250
Method: other: Immobilization Test
Year: 1977 **GLP:** no data
Test substance: no data
Source: Huels AG Marl
Test condition: pH 7.6 - 7.7; 20 - 22 degree C

(21)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC0: = 119
EC50: = 342
EC100: = 638
Method: other: Immobilization Test
Year: 1977 **GLP:** no data
Test substance: no data
Source: Huels AG Marl
Test condition: pH 7.6 - 7.7; 20 degree C

(22)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Microcystis aeruginosa (Algae, blue, cyanobacteria)
Endpoint: biomass
Exposure period: 8 hour(s)
Unit: mg/l **Analytical monitoring:** no
TT : = 205
Method: other: Cell Multiplication Inhibition Test
Year: 1977 **GLP:** no data
Test substance: no data
Remark: TT = toxicity threshold
Source: Huels AG Marl
Test condition: pH 7.0; 27 degree C

(23)

Species: Scenedesmus quadricauda (Algae)
Endpoint: biomass
Exposure period: 8 hour(s)
Unit: mg/l **Analytical monitoring:** no
TT : = 80
Method: other: Cell Multiplication Inhibition Test
Year: 1978 **GLP:** no data
Test substance: no data
Remark: TT = toxicity threshold
Source: Huels AG Marl
Test condition: pH 7.0; 27 degree C

(24)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: Chilomonas paramaecium (Protozoa)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
TT : = 600
Method: other: Cell Multiplication Inhibition Test
Year: 1980 **GLP:** no data
Test substance: no data
Remark: TT = toxicity threshold
Source: Huels AG Marl
Test condition: pH 6.9; 20 degree C

(25)

Type: aquatic
Species: Entosiphon sulcatum (Protozoa)
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** no
TT : = 411
Method: other: Cell Multiplication Inhibition Test
Year: 1978 **GLP:** no data
Test substance: no data
Remark: TT = toxicity threshold
Source: Huels AG Marl
Test condition: pH 6.9; 25 degree C

(26)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 16 hour(s)
Unit: mg/l **Analytical monitoring:** no
TT : = 200
Method: other: Cell Multiplication Inhibition Test
Year: 1977 **GLP:** no data
Test substance: no data
Remark: TT = toxicity threshold
Source: Huels AG Marl
Test condition: pH 7.0; 25 degree C

(24)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 18 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC10: = 487
Method: other: Pseudomonas–Zellvermehrungs–Hemmtest, DIN 38412 Teil 8, zum Gelbdruck verabschiedet, Bestimmung der Hemmwirkung von Wasserinhaltsstoffen auf Bakterien
Year: **GLP:** no
Test substance: as prescribed by 1.1 – 1.4
Source: Huels AG Marl

(14)

Type: aquatic
Species: Uronema parduzci (Protozoa)
Exposure period: 20 hour(s)
Unit: mg/l **Analytical monitoring:** no
TT : = 727
Method: other: Cell Multiplication Inhibition Test
Year: 1978 **GLP:** no data
Test substance: no data
Remark: TT = toxicity threshold
Source: Huels AG Marl
Test condition: pH 6.9; 25 degree C

(27)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

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4.5.2 Chronic Toxicity to Aquatic Invertebrates

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TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

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4.6.2 Toxicity to Terrestrial Plants

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4.6.3 Toxicity to other Non–Mamm. Terrestrial Species

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4.7 Biological Effects Monitoring

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4.8 Biotransformation and Kinetics

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4.9 Additional Remarks

Remark: Narcotic threshold concentration for tadpoles (Rana pipiens): 697 mg/l of water (concentration at which touching the tadpoles failed to cause motion).

Source: Huels AG Marl

(28)

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 13400 mg/kg bw
Method: other: nicht bekannt
Year: 1974 **GLP:** no data
Test substance: no data
Source: NEUBER GES.M.B.H. WIEN

(29)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 13400 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1962 **GLP:** no
Test substance: no data
Remark: observation period: 14 d
Source: Huels AG Marl

(30)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: > 3200 mg/kg bw
Method: other: Eastman Kodak Company Laboratory of Medicine Protocol.
Year: 1956 **GLP:** no
Test substance: no data
Remark: The test material was administered as a 10 % corn oil solution to five animals at dose levels ranging from 400 to 6400 mg/kg body weight. One rat was used at each dose level. Rats were observed for 14 days; no necropsies were performed.
The approximate oral LD50 was between 3200 and 6400 mg/kg. Weakness, ataxia, and shaking were observed in animals receiving 6400 mg/kg.
Source: Huels AG Marl

(31)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: = 4763 mg/kg bw
Method: other: Acute Oral Toxicity
Year: **GLP:** no
Test substance: no data
Remark: observation period: 24 h
Source: Huels AG Marl

(32)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value: > 13.24 mg/l
Method: other: Eastman Kodak Company Laboratory of Industrial Medicine Protocol
Year: 1956 **GLP:** no
Test substance: no data
Remark: Groups of 3 rats were exposed to an atmosphere containing the aerosolised test material at a concentration of 13.24 mg/l (2790 ppm) for 6 hours or 101.05 mg/l (21,301 ppm) for 2 hours and 5 minutes. Duration of exposure at the high concentration was limited by mortality of the test animals.

The exposure was based on nominal concentrations.

No deaths occurred at the low dose and animals gained weight normally during the 14-day post-exposure observation period. The high dose was lethal; accelerated respiration, loss of coordination, prostration, labored breathing and narcosis were observed in all animals prior to death. The approximate LC50 was between 13.24 mg/l and 101.05 mg/l.
Source: Huels AG Marl

(31)

Type: LC50
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value: > 14.72 mg/l
Method: other: Eastman Kodak Company Laboratory of Industrial Medicine Protocol
Year: 1956 **GLP:** no
Test substance: no data
Remark: Groups of 3 rats were exposed to an atmosphere containing the aerosolised test material at a concentration of 14.72 mg/l (3102 ppm) for 6 hours or 109.0 mg/l (22,977 ppm) for 2 hours and 29 minutes. Duration of exposure at the high concentration was limited by mortality of the test animals.

The exposure was based on nominal concentrations.

No deaths occurred at the low dose and animals gained weight normally during the 14-day post-exposure observation period. The high dose was lethal; prostration and narcosis were observed prior to death. The approximate LC50 was between 14.72 mg/l and 109.0 mg/l.
Source: Huels AG Marl

(31)

Type: LCLo
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 4 hour(s)
Value: = 8000 ppm
Method: other: nicht bekannt
Year: 1962 **GLP:** no data
Test substance: no data
Source: NEUBER GES.M.B.H. WIEN

(33)

Type: LCLo
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 4 hour(s)
Value: = 8000 ppm
Method: other: see reference
Year: 1962 **GLP:** no
Test substance: no data
Remark: details not reported
Source: Huels AG Marl

(30)

Type: other: LT0
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time:
Value:
Method: other: see remark
Year: 1962 **GLP:** no
Test substance: no data
Remark: concentrated vapour inhalation; maximal inhalation period for no death: 1 h; observation period: 14 d
no further details reported
Source: Huels AG Marl

(30)

Type: other: see remark
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 4 hour(s)
Value:
Method: other: see reference
Year: 1962 **GLP:** no
Test substance: no data
Remark: mortality:
37.6 mg/l: 4/6
75.2 mg/l: 6/6
observation period: 14 d
no further details reported
Source: Huels AG Marl

(30)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: > 17400 mg/kg bw
Method: other: According to 24-hour cuff method of Draize et al.
Year: 1944 **GLP:** no
Test substance: no data
Remark: contact period: 24 h; observation period: 14 d
Source: Huels AG Marl

(30)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: > 5000 mg/kg bw
Method: other: no data
Year: **GLP:** no data
Test substance: no data
Source: Huels AG Marl

(34)

5.1.4 Acute Toxicity, other Routes

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5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: moderately irritating
EC classificat.: not irritating
Method: Draize Test
Year: 1978 **GLP:** no data
Test substance: no data
Source: NEUBER GES.M.B.H. WIEN

(35)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other: see reference
Year: **GLP:** no
Test substance: no data
Remark: uncovered application of 0.01 ml isobutyl acetate to the clipped skin of 5 albino rabbits was not irritating (observation period: 24 hours); no further details reported
Source: Huels AG Marl

(30)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: moderately irritating
EC classificat.: not irritating
Method: Draize Test
Year: 1978 **GLP:** no data
Test substance: no data
Source: NEUBER GES.M.B.H. WIEN

(36)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method: other: see remark
Year: 1946 **GLP:** no
Test substance: no data
Remark: application of 0.005 – 0.5 ml isobutyl acetate to the center of the cornea; examination after 18 – 24 h; injury grade 2 of 10; no further details reported.
Source: Huels AG Marl

(30)

5.3 Sensitization

Type: Guinea pig maximization test
Species: guinea pig
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method: OECD Guide–line 406 "Skin Sensitization"
Year: 1981 **GLP:** no
Test substance: as prescribed by 1.1 – 1.4
Source: Huels AG Marl

(37)

5.4 Repeated Dose Toxicity

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5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: up to 5000 ug/ml
Metabolic activation: with and without
Result: negative
Method: other: according to Ames et al., Mutat. Res. 31, 347–364
Year: 1975 **GLP:** no
Test substance: as prescribed by 1.1 – 1.4
Source: Huels AG Marl

(38)

5.6 Genetic Toxicity 'in Vivo'

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5.7 Carcinogenicity

–

5.8 Toxicity to Reproduction

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5.9 Developmental Toxicity/Teratogenicity

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5.10 Other Relevant Information

Type: Cytotoxicity
Remark: In vitro incubation of Ehrlich–Landschuetz diploid (ELD) ascites tumour cells with 50 or 100 mg isobutyl acetate/l up to 5 h did not cause increased cell death.
Source: Huels AG Marl

(39)

Type: Metabolism
Remark: Hydrolysis rate of isobutyl acetate in rat ethmoturbinate S9 homogenate: 67 nmol/mg S9 protein/min.
Source: Huels AG Marl

(40)

Type: Neurotoxicity
Remark: Oral narcotic dose for rabbits ED50 = 4299 mg/kg b.w.
Source: Huels AG Marl

(28)

Type: other: see remark
Remark: Upper–respiratory–tract irritation in mice, RD50 = 3890 mg/m3 (concentration causing 50 % reduction of the respiratory rate).
Source: Huels AG Marl

(41)

5.11 Experience with Human Exposure

Remark: Es liegen keine Untersuchungsberichte der BASF vor.
Source: BASF AG Ludwigshafen

(1) Chemline (1992)

(2) TRGS 900 (1993)

(3) 1992-1993 Threshold Limit Values and Biological Exposure Indices - ACGIH
OSHA

(4) ACGIH-Threshold Limit Values (1993-1994)

(5) Huels AG: Emissionserklaerung 1992 (confidential)

(6) Bundesminister des Innern (1990): Gemeinsames Ministerialblatt Nr. 8 (23.03.1990).

(7) Stoerfall-Verordnung vom 20.09.1991

(8) Huels AG: Sicherheitsdatenblatt "Isobutylacetat 98/100 %", Version 05, 25 Feb. 1997

(9) Stoerfallverordnung vom 20.09.1991

(10) Eastman Chemical Company: Material Safety Data Sheet "Isobutyl acetate", approval date 31.07.1992

(11) Sicherheitsdatenblatt Huels AG vom 14.03.94

(12) BASF AG, Sicherheitsdatenblatt Isobutylacetat (29.03.1994)

(13) BASF AG, Sicherheitsdatenblatt "Isobutylacetat" (29.04.1994)

(14) Huels-Untersuchung (unveroeffentlicht)

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7.1 Risk Assessment

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