

SAFETY DATA SHEET



Isobutyric acid
10290

Version / Revision
Supersedes Version

2.01
2.00***

Revision Date
Issuing date

31-Jan-2019
31-Jan-2019

SECTION 1: Identification of the substance / mixture and of the company / undertaking

1.1. Product identifier

Identification of the
substance/preparation

Isobutyric acid

CAS-No
EC No.

79-31-2
201-195-7

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the Substance /
Preparation

Intermediate.

Uses advised against

None

1.3. Details of the supplier of the safety data sheet

Company/Undertaking
Identification

OXEA GmbH
Rheinpromenade 4A
D-40789 Monheim
Germany

Product Information

Product Stewardship
FAX: +49 (0)208 693 2053
email: psq@oxea-chemicals.com

1.4. Emergency telephone number

Emergency telephone number +44 (0) 1235 239 670 (UK) available 24/7***
in USA, call 800 424 9300
outside USA, call +1.703.527.3887, collect calls accepted

SECTION 2: Hazards identification

Europe

2.1. Classification of the substance or mixture

This substance is classified based on Directive 1272/2008/EC and its amendments (CLP Regulation)

Flammable liquid Category 3, H226***
Acute oral toxicity Category 4, H302***
Acute dermal toxicity Category 3, H311***
Skin corrosion/irritation Category 1B, H314***
Serious eye damage/eye irritation Category 1, H318***

Additional information

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For full text of Hazard- and EU Hazard-statements see SECTION 16.***

2.2. Label elements

Labelling according to Regulation 1272/2008/EC and its amendments (CLP Regulation).***

Hazard pictograms



Signal word

Danger

Hazard statements

H226: Flammable liquid and vapour.
H302: Harmful if swallowed.
H311: Toxic in contact with skin.
H314: Causes severe skin burns and eye damage.

Precautionary statements

P280: Wear protective gloves/protective clothing/eye protection/face protection.
P301 + P330 + P331: IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P304 + P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310: Immediately call a POISON CENTER/doctor.

2.3. Other hazards

Vapours may form explosive mixture with air

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin

PBT and vPvB assessment

This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)***

USA

2.1. Classification of the substance or mixture

This substance is classified in accordance with paragraph (d) of §1910.1200 (GHS-US classification).***

Acute dermal toxicity Category 3, H311***
Skin corrosion/irritation Category 1B, H314***
Serious eye damage/eye irritation Category 1, H318***
Flammable liquid Category 3, H226***
Environmental hazard Aquatic Acute 3; H402***

OSHA Specified Hazards

Not applicable.

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2.2. Label elements

Labeling according to §1910.1200 (GHS-US labeling).***

Hazard symbol(s) ***



Signal word

Danger***

Hazard statements

H226: Flammable liquid and vapor.
H311: Toxic in contact with skin.
H314: Causes severe skin burns and eye damage.
H402: Harmful to aquatic life***

Precautionary statements

Prevention

P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233: Keep container tightly closed.
P240: Ground and bond container and receiving equipment.
P241: Use explosion-proof electrical/ ventilating/ lighting equipment.
P242: Use non-sparking tools.
P243: Take action to prevent static discharges.
P280: Wear protective gloves/protective clothing/eye protection/face protection.
P260: Do not breathe gas/mist/vapours.
P264: Wash hands thoroughly after handling.
P273: Avoid release to the environment.***

Response

P301 + P330 + P331: IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P302 + P352: IF ON SKIN: Wash with plenty of soap and water.
P361: Take off immediately all contaminated clothing and wash it before reuse.
P304 + P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P310: Immediately call a POISON CENTER/doctor.
P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.***

Storage

P403 + P235: Store in a well ventilated place. Keep cool.
P405: Store locked up.***

Disposal

P501: Dispose of contents/container in accordance with local regulation.***

2.3. Other hazards

Vapours may form explosive mixture with air

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin***

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SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	REACH-No	1272/2008/EC	Concentration (%)
Isobutyric acid	79-31-2	01-2119488973-18** *	Flam. Liq. 3; H226 Acute Tox. 4; H302 Acute Tox. 3; H311 Skin Corr. 1B; H314 Eye Dam. 1; H318***	> 99,5

SECTION 4: First aid measures

4.1. Description of first aid measures

Inhalation

Keep at rest. Aerate with fresh air. When symptoms persist or in all cases of doubt seek medical advice.

Eyes

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses. Immediate medical attention is required.

Skin

Wash off immediately with soap and plenty of water. When symptoms persist or in all cases of doubt seek medical advice.

Ingestion

Call a physician immediately. Do not induce vomiting without medical advice.

4.2. Most important symptoms and effects, both acute and delayed

Main symptoms

cough, abdominal pain, vomiting, shortness of breath, unconsciousness, discomfort.

Special hazard

Lung irritation, Lung oedema, Stomach perforation.

4.3. Indication of any immediate medical attention and special treatment needed

General advice

Remove contaminated, soaked clothing immediately and dispose of safely. First aider needs to protect himself.

Treat symptomatically. If ingested, flush stomach and compensate acidosis.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

foam, dry chemical, carbon dioxide (CO₂), water spray

Unsuitable Extinguishing Media

Do not use a solid water stream as it may scatter and spread fire.

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5.2. Special hazards arising from the substance or mixture

Under conditions giving incomplete combustion, hazardous gases produced may consist of:

carbon monoxide (CO)

carbon dioxide (CO₂)

Combustion gases of organic materials must in principle be graded as inhalation poisons

Vapours are heavier than air and may spread along floors

Vapours may form explosive mixture with air

5.3. Advice for firefighters

Special protective equipment for firefighters

Fire fighter protection should include a self-contained breathing apparatus (NIOSH-approved or EN 133) and full fire-fighting turn out gear.

Precautions for firefighting

Cool containers / tanks with water spray. Water run-off and vapor cloud may be corrosive. Dike and collect water used to fight fire. Keep people away from and upwind of fire.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel: For personal protective equipment see section 8. Avoid contact with skin and eyes. Avoid breathing vapors or mists. Keep people away from and upwind of spill/leak. Ensure adequate ventilation, especially in confined areas. Keep away from heat and sources of ignition.

For emergency responders: Personal protection see section 8.***

6.2. Environmental precautions

Prevent further leakage or spillage. Do not discharge product into the aquatic environment without pretreatment (biological treatment plant).

6.3. Methods and material for containment and cleaning up

Methods for containment

Stop the flow of material, if possible without risk. Dike spilled material, where this is possible.

Methods for cleaning up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. If liquid has been spilt in large quantities clean up promptly by scoop or vacuum. Dispose of in accordance with local regulations. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours).

6.4. Reference to other sections

For personal protective equipment see section 8.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product. Provide sufficient air exchange and/or exhaust in work rooms.

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Hygiene measures

When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Advice on the protection of the environment

See Section 8: Environmental exposure controls.

Incompatible products

bases
amines
strong oxidizing agents

7.2. Conditions for safe storage, including any incompatibilities

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours). In case of fire, emergency cooling with water spray should be available. Ground and bond containers when transferring material. Vapours may form explosive mixture with air.***

Technical measures/Storage conditions

Keep containers tightly closed in a cool, well-ventilated place. Handle and open container with care. Keep at temperatures between -18 °C and 38 °C (0 °F and 100 °F).

Suitable material

stainless steel, Polyethylene

Unsuitable material

iron

Temperature class

T1

7.3. Specific end use(s)

Intermediate under non-strictly controlled conditions
Distribution of substance***

SECTION 8: Exposure controls / personal protection

8.1. Control parameters

Exposure limits European Union

No exposure limits established.

Exposure limits Germany

No exposure limits established.

Exposure limits United States of America

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No exposure limits established regarding ACGIH, OSHA Z-1 and OSHA Z-2.***

8.2. Exposure controls

Appropriate Engineering controls

General or dilution ventilation is frequently insufficient as the sole means of controlling employee exposure. Local ventilation is usually preferred. Explosion-proof equipment (for example fans, switches, and grounded ducts) should be used in mechanical ventilation systems.

Personal protective equipment

General industrial hygiene practice

Avoid contact with skin, eyes and clothing. Do not breathe vapours or spray mist. Ensure that eyewash stations and safety showers are close to the workstation location.

Hygiene measures

When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Eye protection

Tightly fitting safety goggles. In addition to goggles, wear a face shield if there is a reasonable chance for splash to the face.

Hand protection

Wear protective gloves. Recommendations are listed below. Other protective material may be used, depending on the situation, if adequate degradation and permeation data is available. If other chemicals are used in conjunction with this chemical, material selection should be based on protection for all chemicals present.

Suitable material	butyl-rubber
Evaluation	according to EN 374: level 6
Glove thickness	approx 0,7 mm
Break through time	approx 480 min

Suitable material	nitrile rubber
Evaluation	according to EN 374: level 6
Glove thickness	approx 0,55 mm
Break through time	> 480 min

Skin and body protection

Impervious clothing. Wear face-shield and protective suit for abnormal processing problems.

Respiratory protection

Respirator with filter for organic vapour. Use the indicated respiratory protection if the occupational exposure limit is exceeded and/or in case of product release (dust). Equipment should conform to NIOSH, EN or other applicable national standards.

Environmental exposure controls

Use product only in closed system. If leakage can not be prevented, the substance needs to be suck off at the emersion point, if possible without danger. Observe the exposure limits, clean exhaust air if needed. If recycling is not practicable, dispose of in compliance with local regulations. Inform the responsible authorities in case of leakage into the atmosphere, or of entry into waterways, soil or drains.***

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

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Appearance	liquid				
Colour	colourless				
Odour	pungent				
Odour threshold	8,1 ppm				
pH	2,3 (50 % in water @ 25 °C (77 °F))				
Melting point/range	-64 °C (Pour point)				
Boiling point/range	156 °C				
Flash point	56 - 62 °C				
Method	ISO 2719				
Evaporation rate	No data available				
Flammability (solid, gas)	Does not apply, the substance is a liquid				
Lower explosion limit	1,6 Vol %				
Upper explosion limit	7,3 Vol %				
Vapour pressure	***				
Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
2	0,2***	0,002***	20	68	DIN EN 13016-2***
13	1,3***	0,013***	50	122	DIN EN 13016-2***
Vapour density	3,0 (Air = 1) @ 20 °C (68 °F)				
Relative density	***				
Values	@ °C	@ °F	Method		
0,948	20	68	DIN 51757		
Solubility	618 g/l @ 20 °C, in water, OECD 105***				
log Pow	1,1 (measured), OECD 117				
Autoignition temperature	455 °C				
Method	DIN 51794				
Decomposition temperature	No data available				
Viscosity	1,32 mPa*s @ 20 °C				
Method	DIN 51562, dynamic				
Oxidizing properties	Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties				
Explosive properties	Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties				

9.2. Other information

Molecular weight	88,10
Molecular formula	C4 H8 O2
Refractive index	1,393 @ 20 °C
Surface tension	70,2 mN/m (1 g/l @ 20°C (68°F)), OECD 115

SECTION 10: Stability and Reactivity

10.1. Reactivity

The reactivity of the product corresponds to the typical reactivity shown by the substance group as described in any text book on organic chemistry.

10.2. Chemical stability

Stable under recommended storage conditions.

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10.3. Possibility of hazardous reactions

Vapours may form explosive mixture with air.

10.4. Conditions to avoid

Avoid contact with heat, sparks, open flame and static discharge. Avoid any source of ignition.

10.5. Incompatible materials

bases, amines, strong oxidizing agents.

10.6. Hazardous decomposition products

No decomposition if stored and applied as directed.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Likely routes of exposure Inhalation, Eye contact, Skin contact, Ingestion***

Acute toxicity				
Isobutyric acid (79-31-2)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	2230 mg/kg	rat, male/female	OECD 401
Dermal	LD50	474 mg/kg (24 h)	rabbit	OECD 402
Inhalative	LC0	9,59 mg/l (8 h)	rat, male/female	OECD 403

Isobutyric acid, CAS: 79-31-2

Assessment

The available data lead to the classification given in section 2
Based on available data, the classification criteria are not met for:
Acute oral toxicity
Acute inhalation toxicity***

Irritation and corrosion				
Isobutyric acid (79-31-2)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	corrosive	OECD 404	read across
Eyes	rabbit	corrosive		

Isobutyric acid, CAS: 79-31-2

Assessment

The available data lead to the classification given in section 2
For respiratory irritation, no data are available***

Isobutyric acid, CAS: 79-31-2

Assessment

Based on available data, the classification criteria are not met for:
Skin sensitization
For respiratory sensitization, no data are available***

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Subacute, subchronic and prolonged toxicity				
Isobutyric acid (79-31-2)				
Type	Dose	Species	Method	
Subchronic toxicity	NOAEL: 375 mg/kg/d (90d)	rat, male/female	OECD 408 Oral***	read across
Subchronic toxicity	NOAEL: 2500 ppm	rat, male/female	OECD 413 Inhalation***	read across

Isobutyric acid, CAS: 79-31-2

Assessment

Based on available data, the classification criteria are not met for:
STOT RE***

Carcinogenicity, Mutagenicity, Reproductive toxicity					
Isobutyric acid (79-31-2)					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		CHO (Chinese Hamster Ovary) cells	negative	OECD 476 (Mammalian Gene Mutation)	
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	
Mutagenicity		mouse	negative	OECD 474	read across in vivo***
Reproductive toxicity	NOAEC: 2500 ppm***	rat***		EPA OPPTS 870.3800	read across
Developmental Toxicity	NOEC 11,9 mg/m ³ ***	rat		OECD 414, Inhalative	read across
Developmental Toxicity	NOEC 2,8 mg/m ³ ***	rabbit	Maternal toxicity	OECD 414, Inhalative	read across
Developmental Toxicity	NOEC 2,8 mg/m ³ ***	rabbit	Fetal toxicity, Embryotoxicity	OECD 414, Inhalative	read across
Developmental Toxicity	NOEC 11,9 mg/m ³ ***	rabbit	Teratogenicity	OECD 414, Inhalative	read across

Isobutyric acid, CAS: 79-31-2

CMR Classification

The available data on CMR properties are summarized in the table above. They do not indicate a classification into categories 1A or 1B***

Evaluation

In vitro tests did not show mutagenic effects
Did not show mutagenic effects in animal experiments
In the absence of specific alerts no cancer testing is required***

Isobutyric acid, CAS: 79-31-2

Main symptoms

cough, abdominal pain, vomiting, shortness of breath, unconsciousness, discomfort.

Target Organ Systemic Toxicant - Single exposure

Based on available data, the classification criteria are not met for:
STOT SE***

Target Organ Systemic Toxicant - Repeated exposure

Based on available data, the classification criteria are not met for:
STOT RE***

Aspiration toxicity

Due to the viscosity, this product does not present an aspiration hazard***

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Other adverse effects

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin.

Note

Handle in accordance with good industrial hygiene and safety practice. Further details on substance data can be found in the registration dossier under the following link:

<http://echa.europa.eu/information-on-chemicals/registered-substances>.***

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity			
Isobutyric acid (79-31-2)			
Species	Exposure time	Dose	Method
Daphnia magna (Water flea)	48h	EC50: 51,25 mg/l	DIN 38412, part 11
Desmodesmus subspicatus	72h	EC50: 45,1 mg/l (Biomass)	DIN 38412, part 9
Leuciscus idus (Golden orfe)	96h	LC50: 146,6 mg/l	DIN 38412, part 15
Tetrahymena pyriformis	40 h	IC50: 190 mg/l (Growth inhibition)	

12.2. Persistence and degradability

Isobutyric acid, CAS: 79-31-2

Biodegradation

> 95 % (10 d), activated sludge, non-adapted, aerobic, OECD 302 B (Zahn-Wellens Test).

Abiotic Degradation		
Isobutyric acid (79-31-2)		
Type	Result	Method
Hydrolysis***	not expected***	
Photolysis***	No data available***	

12.3. Bioaccumulative potential

Isobutyric acid (79-31-2)		
Type	Result	Method
log Pow***	1,1***	measured, OECD 117***
log BCF***	0,5***	calculated***

12.4. Mobility in soil

Isobutyric acid (79-31-2)		
Type	Result	Method
Surface tension***	70,2 mN/m (1 g/l @ 20°C (68°F))***	OECD 115***
Adsorption/Desorption***	log Koc: 1,65***	calculated***
Distribution to environmental compartments***	Air: 7,39 % Soil: 55 % Water: 37,5 % Sediment: 0,07 %***	calculated Fugacity Model Level III***

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12.5. Results of PBT and vPvB assessment

Isobutyric acid, CAS: 79-31-2

PBT and vPvB assessment

This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)**

12.6. Other adverse effects

Isobutyric acid, CAS: 79-31-2

No data available**

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product Information

Disposal required in compliance with all waste management related state and local regulations. The choice of the appropriate method of disposal depends on the product composition by the time of disposal as well as the local statutes and possibilities for disposal.

Hazardous waste according to European Waste Catalogue (EWC)

Uncleaned empty packaging

Contaminated packaging should be emptied as far as possible and after appropriate cleansing may be taken for reuse.

SECTION 14: Transport information

ICAO-TI / IATA-DGR

14.1. UN number

*** UN 2529

14.2. UN proper shipping name

*** Isobutyric acid***

14.3. Transport hazard class(es)

*** 3

Subsidiary Risk

8***

14.4. Packing group

*** III

14.5. Environmental hazards

no***

14.6. Special precautions for user

no data available***

IMDG

14.1. UN number

*** UN 2529

14.2. UN proper shipping name

*** Isobutyric acid***

14.3. Transport hazard class(es)

*** 3

Subsidiary Risk

8***

14.4. Packing group

*** III

14.5. Environmental hazards

no***

14.6. Special precautions for user

EmS

F-E, S-C

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14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code not applicable***

ADR/RID

14.1. UN number *** UN 2529
14.2. UN proper shipping name *** Isobutyric acid
14.3. Transport hazard class(es) *** 3
Subsidiary Risk 8***
14.4. Packing group *** III
14.5. Environmental hazards no***
14.6. Special precautions for user ***
ADR Tunnel restriction code (D/E)
Classification Code FC
Hazard Number 38

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulation 1272/2008, Annex VI

Isobutyric acid, CAS: 79-31-2

Classification Acute Tox. 4*; H312
Acute Tox. 4*; H302***
Hazard pictograms GHS07 Exclamation mark***
Signal word Warning
Hazard statements H312, H302

DI 2012/18/EU (Seveso III) ***

Category Annex I, part 1:
P5a - c; depending on conditions***

DI 1999/13/EC (VOC Guideline)

Component	Status
Isobutyric acid CAS: 79-31-2	regulated***

International Inventories

Isobutyric acid, CAS: 79-31-2

AICS (AU)***
DSL (CA)***
IECSC (CN)***
EC-No. 2011957 (EU)***
ENCS (2)-608 (JP)***
ISHL (2)-608 (JP)***

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KECI KE-24875 (KR)***
INSQ (MX)***
PICCS (PH)***
TSCA (US)***
NZIoC (NZ)***
TCSI (TW)***

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3

H226: Flammable liquid and vapour.
H302: Harmful if swallowed.
H311: Toxic in contact with skin.
H314: Causes severe skin burns and eye damage.
H318: Causes serious eye damage.***

Abbreviations

A table of terms and abbreviations can be found under the following link:
http://echa.europa.eu/documents/10162/13632/information_requirements_r20_en.pdf

Training advice

For effective first-aid, special training / education is needed.

Sources of key data used to compile the datasheet

Information contained in this safety data sheet is based on Oxea owned data and public sources deemed valid or acceptable. The absence of data elements required by OSHA, ANSI or Annex II, Regulation 1907/2006/EC indicates, that no data meeting these requirements is available.

Further information for the safety data sheet

Changes against the previous version are marked by ***. Observe national and local legal requirements. For more information, other material safety data sheets or technical data sheets please consult the Oxea homepage (www.oxea-chemicals.com).

Disclaimer

For industrial use only. The information contained herein is accurate to the best of our knowledge. We do not suggest or guarantee that any hazards listed herein are the only ones which exist. Oxea makes no warranty of any kind, express or implied, concerning the safe use of this material in your process or in combination with other substances. User has the sole responsibility to determine the suitability of the materials for any use and the manner of use contemplated. User must meet all applicable safety and health standards.

End of Safety Data Sheet