

SAFETY DATA SHEET



Isobutyric acid
10290

Version / Revision
Supersedes Version

3.01
3.00***

Revision Date
Issuing date

12-Jan-2022
12-Jan-2022

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 79-31-2
EC No. 201-195-7
Registration number (REACH) 01-2119488973-18

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

Identified uses Intermediate under non-strictly controlled conditions
Distribution of substance
Uses advised against None

1.3. Details of the supplier of the safety data sheet

Company/Undertaking **OQ Chemicals GmbH**
Identification Rheinpromenade 4A
D-40789 Monheim
Germany

Product Information Product Stewardship
FAX: +49 (0)208 693 2053
email: sc.psq@oq.com

1.4. Emergency telephone number

Emergency telephone number +65 3158 1198 (available 24/7)
000800 100 7479 (for domestic shipments only)

SECTION 2: Hazards identification

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

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

2.2. Label elements

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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)

SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	RECh-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

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

SECTION 4: First aid measures

4.1. Description of first aid measures

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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.

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

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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.

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

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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 and 38 °C (0 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 India

No exposure limits established.

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.

Respiratory protection

Respirator with A filter. Full mask with above mentioned filter according to producers using requirements or self-contained breathing apparatus. Equipment should conform to EN 136 or EN 140 and EN 143.

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

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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

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.

Equipment should conform to EN 166

Skin and body protection

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

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

Appearance	liquid
Colour	colourless
Odour	pungent
Odour threshold	8,1 ppm
pH	2,3 (50 % in water @ 25 °C (77 °F)) DIN 19268***
Melting point/range	-64 °C (Freezing Point)***
Boiling point/range	156 °C @ 1013 hPa***
Flash point	56 - 62 °C
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

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log Pow	1,1 (measured), OECD 117
Autoignition temperature	455 °C @ 1018 hPa***
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
log Koc	1,65 calculated***
Dissociation constant	pKa 5 @ 21 °C (69,8 °F) OECD 112***
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.

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

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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 male***	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

Subacute, subchronic and prolonged toxicity

Isobutyric acid (79-31-2)				
Type	Dose	Species	Method	
Subchronic toxicity	NOEL: 375 mg/kg/d (90d)***	rat, male/female	OECD 408 Oral	read across
Subchronic toxicity	NOAEC: 2500 ppm/d (14 weeks)***	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

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Reproductive toxicity	NOAEL: 2500 ppm***	rat		EPA OPPTS 870.3800 Inhalation***	read across
Developmental Toxicity	NOAEL 11,9 mg/l***	rat	Maternal toxicity Fetal toxicity Teratogenicity***	OECD 414, Inhalative	read across***
Developmental Toxicity	NOAEL 3 mg/l***	rabbit	Maternal toxicity	OECD 414, Inhalative	read across
Developmental Toxicity	NOAEL 11,9 mg/l***	rabbit	Teratogenicity Fetal toxicity, Embryotoxicity***	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

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)	

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12.2. Persistence and degradability

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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	Half-life (DT50): 167 h***	

12.3. Bioaccumulative potential

Isobutyric acid (79-31-2)		
Type	Result	Method
log Pow	1,1 @ 25 °C (77 °F)***	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

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)

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

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

International Inventories

Isobutyric acid, CAS: 79-31-2
AICS (AU)

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DSL (CA)
IECSC (CN)
EC-No. 2011957 (EU)
ENCS (2)-608 (JP)
ISHL (2)-608 (JP)
KECI KE-24875 (KR)
INSQ (MX)
PICCS (PH)
TSCA (US)
NZIoC (NZ)**
TCSI (TW)

National regulatory information India

Hazardous Chemicals, Schedule 2: Threshold Quantities at an Isolated Storage
not listed

Hazardous Chemicals, Schedule 3: Threshold Quantities in an Industrial Installation
not listed

For details and further information please refer to the original regulation.

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 OQ 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 OQ homepage (www.chemicals.oq.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. OQ 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