

Chemical Safety Data Sheet MSDS / SDS

Isobutyric acid SDS

Revision Date:2024-04-25 Revision Number:1

Section 1	Section 2	Section 3	Section 4	Section 5	Section 6	Section 7	Section 8
Section 9	Section 10	Section 11	Section 12	Section 13	Section 14	Section 15	Section 16

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

Product name: Isobutyric acid

CAS: 79-31-2

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

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

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SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 4, Oral

Acute toxicity - Category 4, Dermal

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H302 Harmful if swallowed

H312 Harmful in contact with skin

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P317 Get medical help.

P321 Specific treatment (see ... on this label).

P362+P364 Take off contaminated clothing and wash it before reuse.

Storage

none

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	Isobutyric acid
Common names and synonyms:	Isobutyric acid
CAS number:	79-31-2
EC number:	201-195-7
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Give one or two glasses of water to drink. Do NOT induce vomiting. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Inhalation causes irritation of nose and throat. Ingestion causes irritation of mouth and stomach. Contact with eyes or skin causes irritation. (USCG, 1999)

Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean

patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Organic acids and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

Extinguish with dry chemical, alcohol foam, or carbon dioxide.

Specific hazards arising from the chemical

Excerpt from ERG Guide 132 [Flammable Liquids - Corrosive]: Flammable/combustible material. May be ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. (ERG, 2016)

Special protective actions for fire-fighters

Use alcohol-resistant foam, powder, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Remove all ignition sources. Collect leaking and spilled liquid in covered containers as far as possible. Wash away remainder with plenty of water.

Environmental precautions

Remove all ignition sources. Collect leaking and spilled liquid in covered containers as far as possible. Wash away remainder with plenty of water.

Methods and materials for containment and cleaning up

Environmental considerations: Land spill: Dig a pit, pond, lagoon, holding area to contain liquid or solid material. Dike surface flow using soil, sand bags, foamed polyurethane, or foamed concrete. Absorb bulk liquid with fly ash or cement powder. Neutralize with agricultural lime (CaO), crushed limestone (CaCO₃) or sodium bicarbonate (NaHCO₃). SRP: If time permits, pits, ponds, lagoons,

soak holes, or holding areas should be contained with a flexible impermeable membrane liner.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Above 56°C use a closed system, ventilation and explosion-proof electrical equipment. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Fireproof. Separated from strong bases and food and feedstuffs.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear face shield.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid.
Colour:	Colourless, clear.
Odour:	Pungent odor like that of butyric acid, but not as unpleasant
Melting point/freezing point:	-64 °C.
Boiling point or initial boiling point and boiling range:	156 °C. Atm. press.:1 013 hPa.
Flammability:	Flammable. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit:	Lower flammable limit: 2.0% by volume, Upper flammable limit: 9.2% by volume
Flash point:	62 °C. Atm. press.:1 013 hPa.
Auto-ignition temperature:	455 °C. Atm. press.:1 018 hPa.
Decomposition temperature:	no data available
pH:	2.3.
Kinematic viscosity:	dynamic viscosity (in mPa s) = 1.322. Temperature:20°C.
Solubility:	Miscible with water

Partition coefficient n-octanol/water:	Pow = 12.6. Temperature:25 °C.;log Pow = 1.1. Temperature:25 °C.
Vapour pressure:	Ca. 2 hPa. Temperature:20 °C. Remarks:Extrapolated result based on experimental result.
Density and/or relative density:	947.7 kg/m ³ . Temperature:20 °C.
Relative vapour density:	3.04 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

The substance is a weak acid.

Chemical stability

Stable during transport.

Possibility of hazardous reactions

2-Methylpropanoic acid/ is combustible.The vapour is heavier than air.ISOBUTYRIC ACID corrodes aluminum and other metals. Flammable hydrogen gas may accumulate in enclosed spaces in which this reaction has taken place (USCG, 1999).

Conditions to avoid

no data available

Incompatible materials

2-Methylpropanoic acid can react with oxidizing materials.

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - 2 230 mg/kg bw.

Inhalation: LC0 - rat (male/female) - 9.59 mg/L air.

Dermal: LD50 - rabbit (male) - 0.5 mL/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is corrosive to the eyes, skin and respiratory tract. Corrosive on ingestion.

STOT-repeated exposure

no data available

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - *Leuciscus idus* - 146.6 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 51.25 mg/L - 48 h.

Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - 45.1 mg/L - 72 h.

Toxicity to microorganisms: IC50 - *Tetrahymena pyriformis* - 190 mg/L - 40 h.

Persistence and degradability

ANAEROBIC: Isobutyric acid is reported to be susceptible to anaerobic biodegradation(1). Under anaerobic conditions, isobutyric acid was metabolized by an enriched acetate culture cross acclimated with isobutyric acid at a rate of 250 mg/L following a 3 day lag period(2).

Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for isobutyric acid(SRC), using a log Kow of 0.94(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of isobutyric acid is estimated as 77(SRC), using a log Kow of 0.94(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that isobutyric acid is expected to have high mobility in soil. The pKa of isobutyric acid is 4.84(4), indicating that this compound will exist almost entirely in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(5).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN2529 (For reference only, please check.)

IMDG: UN2529 (For reference only, please check.)

IATA: UN2529 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ISOBUTYRIC ACID (For reference only, please check.)

IMDG: ISOBUTYRIC ACID (For reference only, please check.)

IATA: ISOBUTYRIC ACID (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)

IMDG: 3 (For reference only, please check.)

IATA: 3 (For reference only, please check.)

Packing group, if applicable

ADR/RID: III (For reference only, please check.)

IMDG: III (For reference only, please check.)

IATA: III (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website:
<http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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