

## Chemical Safety Data Sheet MSDS / SDS

## Isobutyl isobutyrate SDS

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

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

Product name: Isobutyl isobutyrate

CAS: 97-85-8

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

Relevant identified uses: For R&amp;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**

Flammable liquids, Category 3

Specific target organ toxicity - single exposure, Category 3

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

### GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

### Hazard statement(s)

H226 Flammable liquid and vapour

H336 May cause drowsiness or dizziness

H412 Harmful to aquatic life with long lasting effects

### Precautionary statement(s)

### 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/hearing protection/...

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

P273 Avoid release to the environment.

### Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].

P370+P378 In case of fire: Use ... to extinguish.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P319 Get medical help if you feel unwell.

### Storage

P403+P235 Store in a well-ventilated place. Keep cool.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

## 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:	Isobutyl isobutyrate
Common names and synonyms:	Isobutyl isobutyrate
CAS number:	97-85-8
EC number:	202-612-5
Concentration:	100%

## SECTION 4: First aid measures

### Description of necessary first-aid measures

#### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison

Control Center immediately.

**Most important symptoms/effects, acute and delayed**

Exposure can cause irritation of eyes, nose and throat. Toxic by inhalation. (USCG, 1999)

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

no data available

**SECTION 5: Firefighting measures**

**Suitable extinguishing media**

Extinguishing method: "alcohol" foam

**Specific hazards arising from the chemical**

Special Hazards of Combustion Products: Irritating vapors and toxic gases, such as carbon dioxide and carbon monoxide, may be formed when involved in fire. Behavior in Fire: Vapors can flow along surfaces to distant ignition source and flash back. (USCG, 1999)

**Special protective actions for fire-fighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**SECTION 6: Accidental release measures**

**Personal precautions, protective equipment and emergency procedures**

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

**Environmental precautions**

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

### Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

## SECTION 7: Handling and storage

### Precautions for safe handling

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

## SECTION 8: Exposure controls/personal protection

### Control parameters

#### Occupational Exposure limit values

Component	Isobutyl isobutyrate			
CAS No.	97-85-8			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m <sup>3</sup>	ppm	mg/m <sup>3</sup>
Denmark	100 provisional	?	?	?
	Remarks			

### 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 tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

### Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

### Thermal hazards

no data available

## SECTION 9: Physical and chemical properties and safety characteristics

**Physical state:** Isobutyl isobutyrate is a colorless liquid with a pleasant fruity odor. Moderately toxic by inhalation. Insoluble in water and floats on water, but soluble in alcohol and ethers. It is used as a flavoring and in the manufacture of insecticides.

**Colour:** COLORLESS LIQUID

**Odour:** FRUITY ODOR

**Melting point/freezing point:** -80°C

**Boiling point or initial boiling point and boiling range:** 148°C

**Flammability:** no data available

**Lower and upper explosion limit/flammability limit:** LOWER FLAMMABLE LIMIT: 0.96% BY VOLUME; UPPER FLAMMABLE LIMIT: 7.59% BY VOLUME

Flash point:	40 °C
Auto-ignition temperature:	810 DEG F (432 DEG C)
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	0.5 G PER 100 ML WATER
Partition coefficient n-octanol/water:	no data available
Vapour pressure:	1 mm Hg ( 39.9 °C)
Density and/or relative density:	0.856
Relative vapour density:	4.97 (AIR= 1)
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Highly flammable. Insoluble in water.

### Chemical stability

no data available

### Possibility of hazardous reactions

ISOBUTYL ISOBUTYRATE, [FLAMMABLE LIQUID] reacts with acids to liberate heat along with alcohols and acids. Strong oxidizing acids may cause a vigorous reaction that is sufficiently exothermic to ignite the reaction products. Heat is also generated by the interaction with caustic solutions. Flammable hydrogen is generated by mixing with alkali metals and hydrides.

**Conditions to avoid**

no data available

**Incompatible materials**

It may react with oxidizing material.

**Hazardous decomposition products**

no data available

**SECTION 11: Toxicological information****Acute toxicity**

Oral: no data available

Inhalation: no data available

Dermal: no data available

**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**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

**SECTION 12: Ecological information**

**Toxicity**

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

**Persistence and degradability**

Data specific to the biodegradation of 2-methylpropyl isobutyrate were not located; however, similar aliphatic esters have been shown to biodegrade readily(1-2); therefore, 2-methylpropyl isobutyrate is expected to biodegrade readily(SRC).

**Bioaccumulative potential**

Based upon a water solubility of 1000 mg/L at 20 deg C(1), the BCF for 2-methylpropyl isobutyrate can be estimated to be 12.2 from a recommended linear regression-derived equation(2,SRC). This estimated BCF indicates that bioconcentration in aquatic organisms is not important(SRC).

### **Mobility in soil**

Based upon a water solubility of 1000 mg/L at 20 deg C(1), the Koc for 2-methylpropyl isobutyrate can be estimated to be 98 from a linear regression-derived equation(2, SRC). This Koc estimation indicates high soil mobility(3).

### **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: UN2528 (For reference only, please check.)

IMDG: UN2528 (For reference only, please check.)

IATA: UN2528 (For reference only, please check.)

### **UN Proper Shipping Name**

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

IMDG: ISOBUTYL ISOBUTYRATE (For reference only, please check.)

IATA: ISOBUTYL ISOBUTYRATE (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](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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