

## Chemical Safety Data Sheet MSDS / SDS

## Isobutyronitrile 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: Isobutyronitrile  
CAS: 78-82-0

**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  
Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090  
Telephone: +91 9550333722

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

Flammable liquids, Category 2  
Acute toxicity - Category 3, Oral

Acute toxicity - Category 3, Inhalation

### GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

### Hazard statement(s)

H225 Highly flammable liquid and vapour

H301+H331 Toxic if swallowed or if inhaled

### 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/...

P264 Wash ... thoroughly after handling.

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

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

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

### 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.

P301+P316 IF SWALLOWED: Get emergency medical help immediately.

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

P330 Rinse mouth.

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

P316 Get emergency medical help immediately.

### Storage

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

P405 Store locked up.  
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

#### **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: Isobutyronitrile

Common names and synonyms: Isobutyronitrile

CAS number: 78-82-0

EC number: 201-147-5

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**

Poisonous; may be fatal if inhaled, swallowed, or absorbed through skin. Contact may cause burns to skin and eyes. (Non-Specific - Nitriles) Primarily, they are skin and eye irritants. Large doses cause collapse and stop breathing. (EPA, 1998)

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

First aid & medical therapy should be same as for hcn.

## **SECTION 5: Firefighting measures**

### **Suitable extinguishing media**

Alcohol foam. water may be ineffective.

### **Specific hazards arising from the chemical**

Vapor may explode if ignited in an enclosed area. Toxic oxides of nitrogen are produced during combustion. It is a flammable/combustible material and may be ignited by heat, sparks, or flames. Vapors may travel to a source of ignition and flash back. Container may explode in heat of fire. Vapor explosion and poison hazard indoors, outdoors or in sewers. Runoff to sewer may create fire or explosion hazard. Hazardous polymerization may not occur. (EPA, 1998)

### **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	Isobutyronitrile			
CAS No.	78-82-0			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m <sup>3</sup>	ppm	mg/m <sup>3</sup>
USA - NIOSH	8	22	?	?
	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:	Isobutyronitrile is a clear colorless liquid. Flash point 47°F. Less dense than water. Vapors heavier than air. Toxic oxides of nitrogen produced during combustion.
Colour:	Colorless liquid
Odour:	Almond-like odor.
Melting point/freezing point:	-72°C(lit.)
Boiling point or initial boiling point and boiling range:	108°C
Flammability:	Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F.

Lower and upper explosion limit/flammability limit:	no data available
Flash point:	8°C(lit.)
Auto-ignition temperature:	900 DEG F (482 DEG C)
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	0.551 cP @ 15 deg C; 0.456 cP @ 30 deg
Solubility:	Slight (NIOSH, 2016)
Partition coefficient n-octanol/water:	log Kow = 0.46
Vapour pressure:	100 mm Hg ( 54.4 °C)
Density and/or relative density:	0.76
Relative vapour density:	2.38 (vs air)
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Highly flammable. Slightly soluble in water.

### Chemical stability

no data available

### **Possibility of hazardous reactions**

A very dangerous fire hazard when exposed to heat or flame. ISOBUTYRONITRILE is incompatible with the following: Oxidizers, reducing agents, strong acids & bases (NIOSH, 2016).

### **Conditions to avoid**

no data available

### **Incompatible materials**

Oxidizers, reducing agents, strong acids & bases.

### **Hazardous decomposition products**

When heated to decomposition it emits toxic fumes of NO<sub>x</sub> and CN<sup>-</sup> /nitrogen oxides and cyanides/.

## **SECTION 11: Toxicological information**

### **Acute toxicity**

Oral: LD50 Rat oral 100 mg/kg

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**

Enzyme-catalyzed hydrolysis of nitriles has been shown to proceed by two distinct routes(1,2); a nitrilase transforms the nitriles directly into acids plus ammonium ion, or a nitrile hydratase forms the amide which is hydrolyzed to acid plus ammonium ion by amidase(1,2). 2-Methylpropanenitrile has been shown to biodegrade readily using the Japanese MITI screening test (2 week incubation, 100 ppm concn, activated sludge seed) with theoretical BODs of 53.9-66.3%(3,4). In another study, a mixed microbial culture, isolated from an environment contaminated with organic cyanides and PCBs, utilized 2-methylpropanenitrile as the sole

source of carbon and nitrogen(5). The mixed microbial culture was grown for 48 hrs at pH 7 with 1 g/l of 2-methylpropanenitrile; the final pH and ammonia concn were determined to be 8.21 and 51.6 umol/ml, respectively(5).

#### **Bioaccumulative potential**

An estimated BCF of 3 was calculated for 2-methylpropanenitrile(SRC), using a log Kow of 0.46(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 2-methylpropanenitrile is estimated as 42(SRC), using a measured log Kow of 0.46(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 2-methylpropanenitrile is expected to have very high mobility in soil(SRC).

#### **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: UN2284 (For reference only, please check.)  
IMDG: UN2284 (For reference only, please check.)

IATA: UN2284 (For reference only, please check.)

#### **UN Proper Shipping Name**

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

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

IATA: ISOBUTYRONITRILE (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: II (For reference only, please check.)

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

IATA: II (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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