

## Chemical Safety Data Sheet MSDS / SDS

## 4-isopropylbenzotrile 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: 4-isopropylbenzotrile

CAS: 13816-33-6

**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

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

## GHS label elements, including precautionary statements

Pictogram(s)



Signal word

No signal word

Hazard statement(s)

H411 Toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P273 Avoid release to the environment.

Response

P391 Collect spillage.

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: 4-isopropylbenzotrile

Common names and synonyms: 4-isopropylbenzotrile

CAS number: 13816-33-6

EC number: 237-492-3

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**

no data available

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

no data available

#### **SECTION 5: Firefighting measures**

##### **Suitable extinguishing media**

Use dry chemical, carbon dioxide or alcohol-resistant foam.

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

no data available

### **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

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 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:	Liquid. Liquid.
Colour:	Almost colorless_Pale yellow.
Odour:	no data available

Melting point/freezing point:	> -61 - < -60 °C. Atm. press.:1 013 hPa.
Boiling point or initial boiling point and boiling range:	> 243 - < 245 °C. Atm. press.:1 013 hPa.
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	94 °C. Atm. press.:1 013 hPa.
Auto-ignition temperature:	440 °C. Atm. press.:> 99.1 - ca. 100.7 kPa.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	In water: 149 mg/L. Temperature:20 °C. pH:6.9.
Partition coefficient n-octanol/water:	log Pow = 2.6. Temperature:35 °C. Remarks:Testing performed at 35°C (column temperature), however the values can be considered to represent the values at an unspecified, probably ambient temperature since the HPLC method with reference substances was used.
Vapour pressure:	12 Pa. Temperature:25 °C.
Density and/or relative density:	0.952 g/cm <sup>3</sup> . Temperature:20 °C.
Relative vapour density:	no data available
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

no data available

### Possibility of hazardous reactions

no data available

### Conditions to avoid

no data available

### Incompatible materials

no data available

### Hazardous decomposition products

no data available

## SECTION 11: Toxicological information

### Acute toxicity

Oral: LD50 - rat (male) - 3.9 g/Kg.

Inhalation: no data available

Dermal: LD50 - rabbit (female) - > 5 000 mg/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**

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: EC50 - *Daphnia magna* - 6.13 mg/L - 48 h.

Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - 8.92 mg/L - 72 h.

Toxicity to microorganisms: no data available



**Persistence and degradability**

no data available

**Bioaccumulative potential**

no data available

**Mobility in soil**

no data available

**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: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **UN Proper Shipping Name**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Transport hazard class(es)**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Packing group, if applicable**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Environmental hazards**

ADR/RID: Yes

IMDG: Yes

IATA: Yes

### **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**

Not Listed.

**New Zealand Inventory of Chemicals (NZIoC)**

Listed.

**(PICCS)**

Listed.

**Vietnam National Chemical Inventory**

Listed.

**IECSC)**

Listed.

**Korea Existing Chemicals List (KECL)**

Not 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/>

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any