

## Chemical Safety Data Sheet MSDS / SDS

## Isoprene 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: Isoprene

CAS: 78-79-5

**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

Telephone: +91 9550333722

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

Flammable liquids, Category 1

Germ cell mutagenicity, Category 2

Carcinogenicity, Category 1B  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

### GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

### Hazard statement(s)

H224 Extremely flammable liquid and vapour  
H341 Suspected of causing genetic defects  
H350 May cause cancer  
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/...  
P203 Obtain, read and follow all safety instructions before use.  
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.  
P318 IF exposed or concerned, get medical advice.

#### Storage

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

Common names and synonyms: Isoprene

CAS number: 78-79-5

EC number: 201-143-3

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**

Rinse skin with plenty of water or shower. Remove contaminated clothes. Refer for medical attention .

**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**

Rinse mouth. Do NOT induce vomiting. Refer for medical attention .

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

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: Inhalation or contact with material may irritate or burn skin and eyes. Fire may produce irritating, corrosive and/or toxic gases. Vapors may cause dizziness or suffocation. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

Vapor produces no effects other than slight irritation of the eyes and upper respiratory tract. Liquid may irritate eyes; like gasoline. (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 if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the 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. Aliphatic hydrocarbons and related compounds

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

#### **Suitable extinguishing media**

Use fine spray or fog to control fire by preventing its spread and absorbing some of its heat. Use water spray to keep fire-exposed containers cool. Fight fire from protected location or maximum possible distance.

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

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: HIGHLY FLAMMABLE: Will be easily 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. Substance may be transported hot. For hybrid vehicles, ERG Guide 147 (lithium ion batteries) or ERG Guide 138 (sodium batteries) should also be consulted. If molten aluminum is involved, refer to ERG Guide 169. (ERG, 2016)

Special Hazards of Combustion Products: Toxic vapors are generated when heated Behavior in Fire: May polymerize in containers and explode (USCG, 1999)

#### **Special protective actions for fire-fighters**

Use powder, foam, 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

Evacuate danger area! Consult an expert! Remove all ignition sources. Personal protection: complete protective clothing including self-contained breathing apparatus. Do NOT wash away into sewer. Do NOT let this chemical enter the environment. Collect leaking liquid in sealable containers. Cover the spilled material with inert absorbent. Then store and dispose of according to local regulations.

### Environmental precautions

Evacuate danger area! Consult an expert! Remove all ignition sources. Personal protection: complete protective clothing including self-contained breathing apparatus. Do NOT wash away into sewer. Do NOT let this chemical enter the environment. Collect leaking liquid in sealable containers. Cover the spilled material with inert absorbent. Then store and dispose of according to local regulations.

### Methods and materials for containment and cleaning up

SRP: Wastewater from contaminant suppression, cleaning of protective clothing/equipment, or contaminated sites should be contained and evaluated for subject chemical or decomposition product concentrations. Concentrations shall be lower than applicable environmental discharge or disposal criteria. Alternatively, pretreatment and/or discharge to a POTW is acceptable only after review by the governing authority. Due consideration shall be given to remediation worker exposure (inhalation, dermal and ingestion) as well as fate during treatment, transfer and disposal. If it is not practicable to manage the chemical in this fashion, it must meet Hazardous Material Criteria for disposal.

## SECTION 7: Handling and storage

### Precautions for safe handling

NO open flames, NO sparks and NO smoking. Closed system, ventilation, explosion-proof electrical equipment and lighting. Prevent build-up of electrostatic charges (e.g., by grounding). Do NOT use compressed air for filling, discharging, or 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

Fireproof. Separated from combustible substances, reducing agents, strong oxidants, strong bases, strong acids, alcohols and acid chlorides. Cool. Keep in the dark. Well closed. Store only if stabilized. Provision to contain effluent from fire extinguishing. Store in an area without drain or sewer access. Store in a cool, dry well-ventilated location. Outside or detached storage is preferred. Separate from oxidizing materials.

## SECTION 8: Exposure controls/personal protection

### Control parameters

### Occupational Exposure limit values

MAK: 8.5 mg/m<sup>3</sup>, 3 ppm; peak limitation category: II(8); pregnancy risk group: C; germ cell mutagen group: 5

### 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 safety goggles or eye protection in combination with breathing protection.

#### Skin protection

Protective gloves.

#### Respiratory protection

Use ventilation. Use local exhaust or breathing protection.

#### Thermal hazards

no data available

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

**Physical state:** Isoprene and pentene is a water-white liquid solution of two compounds. Has a faint hydrocarbon odor. Insoluble in water and much less dense than water. Vapors are much heavier than air. May irritate eyes, skin and mucous membranes.

**Colour:** Colorless volatile liquid

Odour:	Mild, aromatic
Melting point/freezing point:	-146°C(lit.)
Boiling point or initial boiling point and boiling range:	34°C(lit.)
Flammability:	Extremely flammable.
Lower and upper explosion limit/flammability limit:	Lower flammable limit: 1.5% by volume; Upper flammable limit: 8.9% by volume
Flash point:	-54°C
Auto-ignition temperature:	428°F
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	0.3 mm <sup>2</sup> /s at 20-25°C
Solubility:	less than 1 mg/mL at 70.7° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Kow = 2.42
Vapour pressure:	8.82 psi ( 20 °C)
Density and/or relative density:	0.681g/mLat 20°C
Relative vapour density:	2.35 (vs air)
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

The substance can readily form explosive peroxides. The substance polymerizes due to heating and under the influence of many materials. This generates fire or explosion hazard. Reacts with strong oxidants, strong reducing agents, strong acids, strong bases, acid chlorides and alcohols. This generates fire and explosion hazard.

### Chemical stability

Unstable, oxidizable

### Possibility of hazardous reactions

Highly flammable, dangerous fire ... risk ... The vapour is heavier than air and may travel along the ground; distant ignition possible. As a result of flow, agitation, etc., electrostatic charges can be generated. Vapours are uninhibited and may polymerize in vents or flame arresters, causing blockage. The unsaturated aliphatic hydrocarbons, such as ISOPRENE and PENTENE, are generally much more reactive than the alkanes. They react vigorously with strong oxidizing agents. Can react exothermically with reducing agents to release gaseous hydrogen. Isoprene readily polymerizes exothermically to form rubber-like products. Pentene inhibits this reaction. Isoprene may undergo autoxidation upon exposure to the air to form explosive peroxides. Violent explosions have occurred at low temperatures in ammonia synthesis gas units. These explosions have been traced to the addition products between dienes (isoprene is a diene) and oxides of nitrogen, produced from the interaction of nitrogen oxide and oxygen. [Bretherick, 1995]. Isoprene oxidize in air to form unstable peroxides that may explode spontaneously [Bretherick, 1979 p.151-154, 164]. Mixing isoprene in equal molar portions with any of the following substances in a closed container caused the temperature and pressure to increase: chlorosulfonic acid, nitric acid(70%), oleum, sulfuric acid (90%) [NFPA 1991].

### Conditions to avoid

no data available

### Incompatible materials

Isoprene (1 g) dissolved in heptane was ozonised at -78 deg C. Soon after cooling was stopped, a violent explosion, followed by a lighter one, occurred. This was attributed to high concn of peroxides and ozonides building up at the rather low temperature employed. Operation at a higher temperature would permit the ozonides and peroxides to decompose, so avoiding high concn in the reaction mixture.

### Hazardous decomposition products

When heated to decomposition, it emits acrid smoke and fumes.



## SECTION 11: Toxicological information

### Acute toxicity

Oral: LD50 Rat oral 2,043-2,210 mg/kg

Inhalation: LC50 Rat inhalation 180 g/cu m/4 hr

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

Evaluation: No epidemiological data relevant to the carcinogenicity of isoprene were available. There is sufficient evidence in experimental animals for the carcinogenicity of isoprene. Overall evaluation: Isoprene is possibly carcinogenic to humans (Group 2B).

### Reproductive toxicity

no data available

### STOT-single exposure

The substance and the vapour are moderately irritating to the eyes, skin and respiratory tract. The substance may cause effects on the central nervous system. This may result in respiratory depression and lowering of consciousness. If swallowed the substance easily enters the airways and could result in aspiration pneumonitis.

### **STOT-repeated exposure**

Repeated or prolonged inhalation may cause effects on the lungs. This substance is possibly carcinogenic to humans. May cause heritable genetic damage to human germ cells.

### **Aspiration hazard**

A harmful contamination of the air can be reached very quickly on evaporation of this substance at 20°C.

## **SECTION 12: Ecological information**

### **Toxicity**

Toxicity to fish: LC50; Species: *Lepomis macrochirus* (Bluegill, length 3.8-6.4 cm, weight 1-2 g); Conditions: freshwater, static, 25 deg C, pH 7.5, hardness 20 mg/L CaCO<sub>3</sub>, alkalinity 18 mg/L CaCO<sub>3</sub>, dissolved oxygen 7.8 mg/L; Concentration: 42540 ug/L for 24 hr (95% confidence interval: 32500-50150 ug/L) /formulated product

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**

AEROBIC: The half-life of isoprene at an initial concentration of 500 ppb in 30 g temperate forest surface soil samples from Ithaca, NY was about 6 hours at temperatures of 5 to 40 deg C. It was also determined that the rate of degradation was slower in subsurface soils (15-18 cm depth) than in surface soil (0-3 cm depth) samples(1).[(1) Cleveland CC, Yavitt JB; Appl Environ Microbiol 64: 172-77 (1998)] Full text: PMC124689

### **Bioaccumulative potential**

BCFs of 5-14 and <5.8-20 were measured in carp (*Cyprinus carpio*) exposed to 50 and 5 ug/L of isoprene over a 6-week period(1). According to a classification scheme(2), these BCFs suggest bioconcentration in aquatic organisms is low(SRC).

### **Mobility in soil**

The Koc of isoprene is estimated as 61(SRC), using a log Kow of 2.42(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that isoprene is expected to have high mobility in soil.

**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: UN1218 (For reference only, please check.)

IMDG: UN1218 (For reference only, please check.)

IATA: UN1218 (For reference only, please check.)

**UN Proper Shipping Name**

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

IMDG: ISOPRENE, STABILIZED (For reference only, please check.)

IATA: ISOPRENE, STABILIZED (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: I (For reference only, please check.)  
IMDG: I (For reference only, please check.)  
IATA: I (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/>

### **Other Information**

Usually contains inhibitors to prevent polymerization. An added stabilizer or inhibitor can influence the toxicological properties of this substance; consult an expert. Check for peroxides prior to distillation; eliminate if found. Do NOT take working clothes home.

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