

## Chemical Safety Data Sheet MSDS / SDS

## 3,5,5-trimethylcyclohex-2-enone 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: 3,5,5-trimethylcyclohex-2-enone

CAS: 78-59-1

**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**

Acute toxicity - Category 4, Oral

Acute toxicity - Category 4, Dermal

Eye irritation, Category 2  
Specific target organ toxicity - single exposure, Category 3  
Carcinogenicity, Category 2

### GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

### Hazard statement(s)

H302 Harmful if swallowed  
H312 Harmful in contact with skin  
H319 Causes serious eye irritation  
H335 May cause respiratory irritation  
H351 Suspected of causing cancer

### 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/...  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P271 Use only outdoors or in a well-ventilated area.  
P203 Obtain, read and follow all safety instructions before use.

### 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.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P319 Get medical help if you feel unwell.

P318 IF exposed or concerned, get medical advice.

#### **Storage**

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: 3,5,5-trimethylcyclohex-2-enone

Common names and synonyms: 3,5,5-trimethylcyclohex-2-enone

CAS number: 78-59-1

EC number: 201-126-0

Concentration: 100%

### **SECTION 4: First aid measures**

#### **Description of necessary first-aid measures**

##### **If inhaled**

Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.

##### **Following skin contact**

Remove contaminated clothes. Rinse and then wash skin with water and soap.

##### **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. Give a slurry of activated charcoal in water to drink. Do NOT induce vomiting.

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

LIQUID: Irritating to skin and eyes. Harmful if swallowed. (USCG, 1999)

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

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary. For contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport. Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal. Ketones and related compounds

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

#### **Suitable extinguishing media**

Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Use "alcohol" foam, dry chemical or carbon dioxide.

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

Combustible. (USCG, 1999)

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

Use water spray, powder, foam, carbon dioxide.

### **SECTION 6: Accidental release measures**

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

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect

leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

#### **Environmental precautions**

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

#### **Methods and materials for containment and cleaning up**

If leak or spill has not ignited, use water spray to disperse vapors & to protect men attempting to stop leak.

### **SECTION 7: Handling and storage**

#### **Precautions for safe handling**

NO open flames. Above 84°C use a closed system and ventilation. 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**

Separated from strong oxidants, strong bases and amines. 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**

TLV: 5 ppm as STEL; A3 (confirmed animal carcinogen with unknown relevance to humans). MAK: 11 mg/m<sup>3</sup>, 2 ppm; peak limitation category: I(2); carcinogen category: 3B; pregnancy risk group: C

#### **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 spectacles.

**Skin protection**

Protective gloves.

**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:	None.
Odour:	Peppermint-like odor
Melting point/freezing point:	-8.1 °C.
Boiling point or initial boiling point and boiling range:	215.3 °C. Atm. press.:1 013 hPa.
Flammability:	Class IIIA Combustible Liquid: Fl.P. at or above 140°F and below 200°F.
Lower and upper explosion limit/flammability limit:	Lower 0.8% by vol; upper 3.8%

Flash point:	85 °C. Atm. press.:Ca. 1 013 hPa.
Auto-ignition temperature:	470 °C. Atm. press.:Ca. 1 013 hPa.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	kinematic viscosity (in mm <sup>2</sup> /s) = 2.83. Temperature:20°C.
Solubility:	0.1 to 1 mg/mL at 64° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Pow = 1.67. Temperature:20 °C. Remarks:PH not reported (not relevant for non-dissociating substance).
Vapour pressure:	0.4 hPa. Temperature:20 °C. Remarks:For values at other temperatures see below.
Density and/or relative density:	921.5 kg/m <sup>3</sup> . Temperature:20 °C.
Relative vapour density:	4.77 (vs air)
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Reacts with strong oxidants, strong bases and amines.

### Chemical stability

no data available

### Possibility of hazardous reactions

Flammable & explosive when exposed to heat or flame. Ketones, such as ISOPHORONE, are reactive with many acids and bases liberating heat and flammable gases (e.g., H<sub>2</sub>). The amount of heat may be sufficient to start a fire in the unreacted portion of the ketone. Ketones react with reducing agents such as hydrides, alkali metals, and nitrides to produce flammable gas (H<sub>2</sub>) and heat.

Ketones are incompatible with isocyanates, aldehydes, cyanides, peroxides, and anhydrides. They react violently with aldehydes, HNO<sub>3</sub>, HNO<sub>3</sub> + H<sub>2</sub>O<sub>2</sub>, and HClO<sub>4</sub>. Forms explosive peroxides

**Conditions to avoid**

no data available

**Incompatible materials**

Incompatible with strong oxidizers

**Hazardous decomposition products**

no data available

**SECTION 11: Toxicological information**

**Acute toxicity**

Oral: LD<sub>50</sub> - rat (male/female) - 1 500 mg/kg bw. Remarks: LD<sub>50</sub>?confidence?limits:?1400-1800?mg/kg.

Inhalation: LC<sub>50</sub> - rat (male) - 7 mg/L air.

Dermal: LD<sub>50</sub> - rabbit (male/female) - 1 200 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**

Cancer Classification: Group C Possible Human Carcinogen

### **Reproductive toxicity**

No studies were located regarding developmental or reproductive effects in humans. (-) Limited evidence in animal studies suggests that isophorone may cause birth defects such as fetal malformations and growth retardation from inhalation exposure to isophorone during pregnancy.

### **STOT-single exposure**

The substance and the vapour are irritating to the eyes and respiratory tract. The substance may cause effects on the central nervous system.

### **STOT-repeated exposure**

no data available

### **Aspiration hazard**

A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20°C.

## **SECTION 12: Ecological information**

### **Toxicity**

Toxicity to fish: LC50 - Pimephales promelas - 228 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: NOEC - Daphnia magna - 15 mg/L - 48 h.

Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - 475 mg/L - 72 h.

Toxicity to microorganisms: EC50 - activated sludge of a predominantly domestic sewage - 100 mg/L - 3 h. Remarks:Respiration rate.

### **Persistence and degradability**

AEROBIC: Isophorone, present at 100 mg/l, reached 3% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/l and the Japanese MITI test(1). Removal of isophorone from unacclimated fresh and salt water seeded with settled domestic wastewater was 42 and 9%, respectively, after 20 days(3). Removal of isophorone from wastewater treated by various different

biological treatment processes: trickling filter, activated sludge, aerated lagoon, and facultative lagoon was 19, 98, 24, and 30%, respectively(4); therefore this compound is not expected to biodegrade rapidly(SRC). A 100% loss was observed when 5 and 10 mg/l isophorone underwent a 7-day static incubation in the dark at 25 deg C under aerobic conditions using settled domestic wastewater as inoculum(2). Using a multi-level respirometric test protocol employing a sludge microbiota, a half-life of 25 days for 100 mg test compound was determined(5).

#### **Bioaccumulative potential**

A BCF of 7 was measured for isophorone in bluegill sunfish(1). The half-life of isophorone in fish tissue was found to be 1 day(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

#### **Mobility in soil**

The Koc of isophorone is estimated as 200(SRC), using a log Kow of 1.7(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that isophorone is expected to have moderate 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: 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: 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**

Not 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

The occupational exposure limit value should not be exceeded during any part of the working exposure.

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