

## Chemical Safety Data Sheet MSDS / SDS

## 3,5,5-trimethylcyclohex-3-en-1-one 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-3-en-1-one

CAS: 471-01-2

**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**

Acute toxicity - Category 4, Oral

Acute toxicity - Category 4, Dermal

Acute toxicity - Category 3, Inhalation  
Specific target organ toxicity - single exposure, Category 3  
Carcinogenicity, Category 2

### GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

### Hazard statement(s)

H302 Harmful if swallowed  
H312 Harmful in contact with skin  
H319 Causes serious eye irritation  
H331 Toxic if inhaled  
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.  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P316 Get emergency medical help immediately.  
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-3-en-1-one

Common names and synonyms: 3,5,5-trimethylcyclohex-3-en-1-one

CAS number: 471-01-2

EC number: 207-434-1

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.
Colour:	No data.
Odour:	no data available
Melting point/freezing point:	-40.7 °C.
Boiling point or initial boiling point and boiling range:	185.5 °C. Atm. press.:1 013.3 hPa. Remarks:Boiling point value calculated value based on vapour pressure measuring.
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	85 °C. Atm. press.:1 013 kPa.
Auto-ignition temperature:	no data available

Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	In water: 0.873 g/L. Temperature:25.
Partition coefficient n-octanol/water:	log Pow = 2.329. Temperature:25 °C.
Vapour pressure:	0.965 hPa. Temperature:23.09 °C. Remarks:Measured value.;7.003 hPa. Temperature:54 °C. Remarks:Measured value.
Density and/or relative density:	0.908. 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/female) - 1 500 mg/kg bw.

Inhalation: LC50 - rat (male) - 7 mg/L air.

Dermal: LD50 - 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**

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: LC50 - Pimephales promelas - 145 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 120 mg/L - 48 h.

Toxicity to algae: no data available

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

**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: no data available

IMDG: no data available

IATA: no data available

### UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

### Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (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**

Not Listed.

**China Catalog of Hazardous chemicals 2015**

Not Listed.

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

Listed.

**(PICCS)**

Not 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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