

## Chemical Safety Data Sheet MSDS / SDS

**4-PENTEN-3-ONE, 5-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)**Revision Date:2023-12-07 Revision Number:1

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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 4-PENTEN-3-ONE, 5-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)  
CBnumber : CB0495785  
CAS : 7779-30-8  
EINECS Number : 231-926-5  
Synonyms : 1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one, 4-PENTEN-3-ONE, 5-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)

**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  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

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

Skin sensitization, Category 1  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

**Label elements****Pictogram(s)**

Signal word : Warning

**Hazard statement(s)**

H317 May cause an allergic skin reaction  
H411 Toxic to aquatic life with long lasting effects

**Precautionary statement(s)****Prevention**

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P272 Contaminated work clothing should not be allowed out of the workplace.  
Chemical Book

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P273 Avoid release to the environment.

#### Response

P302+P352 IF ON SKIN: Wash with plenty of water/...

P333+P317 If skin irritation or rash occurs: Get medical help.

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

P362+P364 Take off contaminated clothing and wash it before reuse.

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

no data available

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## SECTION 3: Composition/information on ingredients

#### Substance

Product name	: 4-PENTEN-3-ONE, 5-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)
Synonyms	: 1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one, 4-PENTEN-3-ONE, 5-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)
CAS	: 7779-30-8
EC number	: 231-926-5
MF	: C <sub>14</sub> H <sub>22</sub> O
MW	: 206.32

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## SECTION 4: First aid measures

#### Description of 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 and effects, both acute and delayed

SYMPTOMS: Symptoms of exposure to this compound may include irritation of the skin and eyes. ACUTE/CHRONIC HAZARDS: This compound is an irritant of the skin and eyes. When heated to decomposition it emits toxic fumes of carbon monoxide and unidentified organic compounds. (NTP, 1992)

## Indication of any immediate medical attention and special treatment needed

no data available

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## SECTION 5: Firefighting measures

### Extinguishing media

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. A water spray may also be used. (NTP, 1992)

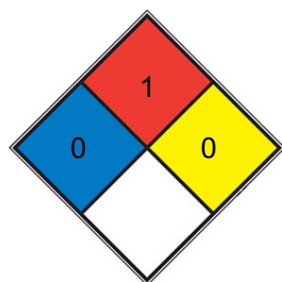
### Specific Hazards Arising from the Chemical

This chemical is probably combustible. (NTP, 1992)

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### NFPA 704



**HEALTH 0** Poses no health hazard, no precautions necessary and would offer no hazard beyond that of ordinary combustible materials

**FIRE 1** Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

**REACT 0** Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

**SPEC.**

**HAZ.**

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## 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.

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## **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.

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## **SECTION 8: Exposure controls/personal protection**

### **Control parameters**

#### **Occupational Exposure limit values**

no data available

#### **Biological limit values**

no data available

### **Exposure 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**

#### **Eye/face protection**

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

#### **Skin protection**

Wear fire/flammable 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

### Information on basic physicochemical properties

Physical state	PHYSICAL DESCRIPTION: Clear, colorless to yellow liquid with a woody, violet odor. (NTP, 1992)
Colour	no data available
Odour	no data available
Melting point/freezing point	-1°C(lit.)
Boiling point or initial boiling point and boiling range	120°C/6.5mmHg(lit.)
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	142°C(lit.)
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	less than 1 mg/mL at 68° F (NTP, 1992)
Partition coefficient n-octanol/water	no data available
Vapour pressure	no data available
Density and/or relative density	0.93
Relative vapour density	greater than 1 (NTP, 1992) (Relative to Air)
Particle characteristics	no data available

## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

no data available

### Possibility of hazardous reactions

1-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)-1-PENTEN-3-ONE is incompatible with strong acids, alkalis or oxidizing agents. (NTP, 1992).

### Conditions to avoid

no data available

### Incompatible materials

no data available

### Hazardous decomposition products

no data available

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## SECTION 11: Toxicological information

### Acute toxicity

- Oral: no data available
- 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

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## 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

no data available

## Bioaccumulative potential

no data available

## Mobility in soil

no data available

## Other adverse effects

no data available

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# 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.

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# SECTION 14: Transport information

## UN Number

ADR/RID: UN2735 (For reference only, please check.)

IMDG: UN2735 (For reference only, please check.)

IATA: UN2735 (For reference only, please check.)

## UN Proper Shipping Name

ADR/RID: AMINES, LIQUID, CORROSIVE, N.O.S. or POLYAMINES, LIQUID, CORROSIVE, N.O.S. (For reference only, please check.)

IMDG: AMINES, LIQUID, CORROSIVE, N.O.S. or POLYAMINES, LIQUID, CORROSIVE, N.O.S. (For reference only, please check.)

IATA: AMINES, LIQUID, CORROSIVE, N.O.S. or POLYAMINES, LIQUID, CORROSIVE, N.O.S. (For reference only, please check.)

## Transport hazard class(es)

ADR/RID: 8 (For reference only, please check.)

IMDG: 8 (For reference only, please check.)

IATA: 8 (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: Yes

IMDG: Yes

IATA: Yes

### **Special precautions for user**

no data available

### **Transport in bulk according to IMO instruments**

no data available

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## **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.

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## **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



ATA: 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?pagelD=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pagelD=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:

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