

## Chemical Safety Data Sheet MSDS / SDS

(1 $\alpha$ ,2 $\beta$ ,5 $\alpha$ )-2,6,6-trimethylbicyclo[3.1.1]heptane SDS

Revision Date:2024-04-25 Revision Number:1

Section 1	Section 2	Section 3	Section 4	Section 5	Section 6	Section 7	Section 8
Section 9	Section 10	Section 11	Section 12	Section 13	Section 14	Section 15	Section 16

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**Product name: (1 $\alpha$ ,2 $\beta$ ,5 $\alpha$ )-2,6,6-trimethylbicyclo[3.1.1]heptane

CAS: 6876-13-7

**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**

Flammable liquids, Category 3

Aspiration hazard, Category 1

## GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

### Hazard statement(s)

H226 Flammable liquid and vapour

H304 May be fatal if swallowed and enters airways

### 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/...

#### 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.

P301+P316 IF SWALLOWED: Get emergency medical help immediately.

P331 Do NOT induce vomiting.

#### 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:	(1 $\alpha$ ,2 $\beta$ ,5 $\alpha$ )-2,6,6-trimethylbicyclo[3.1.1]heptane
Common names and synonyms:	(1 $\alpha$ ,2 $\beta$ ,5 $\alpha$ )-2,6,6-trimethylbicyclo[3.1.1]heptane
CAS number:	6876-13-7
EC number:	229-978-9
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

**SYMPTOMS:** Symptoms of exposure to this compound include irritation of the skin and eyes. It may cause nausea if inhaled. It may also cause eye damage. **ACUTE/CHRONIC HAZARDS:** This chemical may be harmful if swallowed. It may cause irritation of the skin

and eyes. When heated to decomposition it emits toxic fumes of carbon monoxide and carbon dioxide. (NTP, 1992)

#### **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. Turpentine, terpenes, and related compounds

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

#### **Suitable 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 combustible. (NTP, 1992)

#### **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/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 and safety characteristics

Physical state:	PHYSICAL DESCRIPTION: Clear colorless liquid with lint-like particles. Mild odor. (NTP, 1992)
Colour:	Oil
Odour:	no data available
Melting point/freezing point:	-53° C
Boiling point or initial boiling point and boiling range:	157° C at 760 mmHg
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	Lower flammable limit: 0.7% by volume @ 320 deg F (160 deg C); Upper flammable limit: 7.2% by volume @ 320 deg F (160 deg C)
Flash point:	36° C
Auto-ignition temperature:	523° F (NTP, 1992)
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:	log Kow = 4.35 (est)
Vapour pressure:	2 mm Hg at 68° F approximately (NTP, 1992)
Density and/or relative density:	0.857 g/mL at 20°C(lit.)
Relative vapour density:	4.8 approximately (NTP, 1992) (Relative to Air)
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Highly flammable. Insoluble in water.

### Chemical stability

no data available

### Possibility of hazardous reactions

PINANE is incompatible with strong oxidizers. (NTP, 1992)

### Conditions to avoid

no data available

### Incompatible materials

no data available

## **Hazardous decomposition products**

no data available

## **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

**SECTION 12: Ecological information****Toxicity**

Toxicity to fish: LC50; Species: *Oncorhynchus mykiss* (Rainbow trout, larvae); Conditions: freshwater, flow through, 10 deg C, hardness 120 mg/L CaCO<sub>3</sub>; Concentration: 0.0008 ug/L for 60 days /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**

no data available

**Bioaccumulative potential**

An estimated BCF of 450 was calculated for dihydropinene(SRC), using an estimated log Kow of 4.35(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high(SRC), provided the compound is not metabolized by the organism(SRC).

**Mobility in soil**

Using a structure estimation method based on molecular connectivity indices(1), the Koc of dihydropinene can be estimated to be 1,200(SRC). According to a classification scheme(2), this estimated Koc value suggests that dihydropinene is expected to have low 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)**

Not 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/>

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