

## Chemical Safety Data Sheet MSDS / SDS

## Octane-1-thiol 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: Octane-1-thiol

CAS: 111-88-6

**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**

Skin sensitization, Category 1

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

## GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

### Hazard statement(s)

H317 May cause an allergic skin reaction

H410 Very 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.

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 which do not result in classification

no data available

### SECTION 3: Composition/information on ingredients

#### Substance

Chemical name:	Octane-1-thiol
Common names and synonyms:	Octane-1-thiol
CAS number:	111-88-6
EC number:	203-918-1
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 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. Refer for medical attention .

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

Excerpt from ERG Guide 131 [Flammable Liquids - Toxic]: TOXIC; may be fatal if inhaled, ingested or absorbed through skin. Inhalation or contact with some of these materials will irritate or burn skin and eyes. Fire will 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)

#### 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 . Anticipate seizures and treat if necessary . For eye 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 . Cover skin burns with dry sterile dressings after decontamination . Sulfur and related compounds

## SECTION 5: Firefighting measures

### Suitable extinguishing media

Alcohol foam.

### Specific hazards arising from the chemical

Excerpt from ERG Guide 131 [Flammable Liquids - Toxic]: 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 and poison 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. (ERG, 2016)

### Special protective actions for fire-fighters

Use powder, carbon dioxide, foam.

## 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. Do NOT let this chemical enter the environment.

### 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. Do NOT let this chemical enter the environment.

### Methods and materials for containment and cleaning up

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent and remove to safe place. (Extra personal protection: filter respirator for organic gases and vapours.) Do NOT let this chemical enter the environment.

## SECTION 7: Handling and storage

### Precautions for safe handling

NO open flames. Above 69°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

Fireproof. Separated from strong bases, strong acids and oxidants. Fireproof. Separated from strong bases, strong acids and oxidants.

## SECTION 8: Exposure controls/personal protection

### Control parameters

### Occupational Exposure limit values

Component	Octane-1-thiol			
CAS No.	111-88-6			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m <sup>3</sup>	ppm	mg/m <sup>3</sup>
USA - NIOSH	?	?	0,5 (1)	3 (1)
	Remarks			
USA - NIOSH	(1) Ceiling limit value (15 min)			

### 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:	1-octanethiol is a clear colorless liquid. Flash point 115°F. Insoluble in water and less dense than water. Used to make other chemicals.
Colour:	Water-white liquid
Odour:	Mild odor
Melting point/freezing point:	-46°C(lit.)
Boiling point or initial boiling point and boiling range:	200°C(lit.)
Flammability:	Class II Combustible Liquid: Fl.P. at or above 100°F and below 140°F.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	81°C(lit.)

Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	Insoluble (NIOSH, 2016)
Partition coefficient n-octanol/water:	log Kow = 4.2 (est)
Vapour pressure:	0.494mmHg at 25°C
Density and/or relative density:	0.843
Relative vapour density:	5.0 (Air= 1)
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Decomposes on burning. This produces toxic gases including hydrogen sulfide and sulfur oxides. Reacts violently with oxidants. This generates fire hazard. Reacts with strong acids, strong bases and strong reducing agents. Attacks metals and rubber.

### Chemical stability

no data available

### Possibility of hazardous reactions

Combustible 1-OCTANETHIOL is incompatible with the following: Oxidizers, reducing agents, strong acids & bases, alkali metals (NIOSH, 2016).

**Conditions to avoid**

no data available

**Incompatible materials**

Oxidizers, reducing agents, strong acids and bases, alkali metals.

**Hazardous decomposition products**

The substance decomposes on burning producing toxic gases including hydrogen sulfide and sulfur oxides.

**SECTION 11: Toxicological information****Acute toxicity**

Oral: LD50 Rat oral 2000 mg/kg

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**

The substance is mildly irritating to the eyes, skin and respiratory tract. The substance may cause effects on the central nervous system. Exposure at high levels could cause lowering of consciousness.

### **STOT-repeated exposure**

no data available

### **Aspiration hazard**

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

## **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**

Insufficient data are available to determine biodegradability of 1-octanethiol(SRC) but its linear alkyl chemical structure would suggest that biodegradation is important in water(1). 1-Octanethiol, present at 500 mg/L, was not aerobically biodegraded by a pure culture of *Alcaligenes faecalis* over a period of 115-195 hours(2).

### **Bioaccumulative potential**

An estimated BCF of 35 was calculated for 1-octanethiol(SRC), using an estimated log Kow of 4.2(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is moderate(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 1-octanethiol can be estimated to be 930(SRC). According to a classification scheme(2), this estimated Koc value suggests that 1-octanethiol 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: Yes

IMDG: Yes

IATA: Yes

### **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/>

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