

## Chemical Safety Data Sheet MSDS / SDS

## 1-Mercaptooctane

Revision Date:2025-02-01 Revision Number:1

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

## Product identifier

Product name : 1-Mercaptooctane  
CBnumber : CB6852856  
CAS : 111-88-6  
EINECS Number : 203-918-1  
Synonyms : NOM,1-octanethiol

## 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 : 010-86108875

## SECTION 2: Hazards identification

## GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Warning

## Precautionary statements

P501 Dispose of contents/container to....

P405 Store locked up.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P391 Collect spillage. Hazardous to the aquatic environment

P370+P378 In case of fire: Use ... for extinction.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

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

P273 Avoid release to the environment.

P271 Use only outdoors or in a well-ventilated area.  
P270 Do not eat, drink or smoke when using this product.  
P264 Wash skin thoroughly after handling.  
P264 Wash hands thoroughly after handling.  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

#### **Hazard statements**

H410 Very toxic to aquatic life with long lasting effects  
H400 Very toxic to aquatic life  
H373 May cause damage to organs through prolonged or repeated exposure  
H371 May cause damage to organs  
H335 May cause respiratory irritation  
H332 Harmful if inhaled  
H319 Causes serious eye irritation  
H317 May cause an allergic skin reaction  
H315 Causes skin irritation  
H227 Combustible liquid

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: 1-Mercaptooctane
Synonyms	: NOM, 1-octanethiol
CAS	: 111-88-6
EC number	: 203-918-1
MF	: C <sub>8</sub> H <sub>18</sub> S
MW	: 146.29

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## SECTION 4: First aid measures

### **Description of first aid measures**

#### **General advice**

Consult a physician. Show this material safety data sheet to the doctor in attendance.

#### **If inhaled**

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### **In case of skin contact**

Wash off with soap and plenty of water. Consult a physician.

#### **In case of eye contact**

Flush eyes with water as a precaution.

#### **If swallowed**

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

#### Unsuitable extinguishing media

Do NOT use water jet.

### Special hazards arising from the substance or mixture

Carbon oxides Sulfur oxides Combustible.

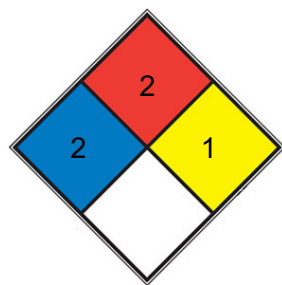
### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### Further information

Use water spray to cool unopened containers.

### NFPA 704



**HEALTH** 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

**FIRE** 2 Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

**REACT** 1 Normally stable, but can become unstable at elevated temperatures and pressures (e.g. [propene](#))

**SPEC.**

**HAZ.**

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## SECTION 6: Accidental release measures

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

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

### **Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.

### **Reference to other sections**

For disposal see section 13.

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

### **Precautions for safe handling**

#### **Advice on safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

#### **Advice on protection against fire and explosion**

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

#### **Hygiene measures**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

For precautions see section 2.2.

### **Conditions for safe storage, including any incompatibilities**

#### **Storage conditions**

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Store in cool place.

#### **Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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

### **control parameter**

#### **Hazard composition and occupational exposure limits**

Does not contain substances with occupational exposure limits.

## Exposure controls

### Personal protective equipment

#### Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

#### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact

with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,4 mm Break through time: 480 min

Material tested: Camatril? (KCL 730 / Aldrich Z677442, Size M)

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 60 min

Material tested: Dermatril? (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

#### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	liquid
Odour	No data available
Odour Threshold	0.0016ppm
pH	No data available
Melting point/freezing point	-49 °C

Initial boiling point and boiling range	197 - 200 °C - lit.
Flash point	70 °C - c.c.
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	0.3 hPa (20 °C)
Vapour density	No data available
Relative density	0.843 (20/4 °C)
Water solubility	0.004g/l
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available

#### Other safety information

No data available

## SECTION 10: Stability and reactivity

#### Reactivity

No data available

#### Chemical stability

Stable under recommended storage conditions. Stable under recommended storage conditions.

#### Possibility of hazardous reactions

No data available

#### Conditions to avoid

Heat, flames and sparks. Heat, flames and sparks.

#### Incompatible materials

Strong oxidizing agents, Strong acids, Alkali metals

#### Hazardous decomposition products

In the event of fire: see section 5

## SECTION 11: Toxicological information

#### Information on toxicological effects

**Acute toxicity**

LD50 Oral - Rat - male and female - 2.436 mg/kg (OECD Test Guideline 420)

LC50 Inhalation - Rat - male and female - 4,5 h - > 3,1 mg/l (OECD Test Guideline 403)

LD50 Dermal - Rabbit - male and female - > 1.680 mg/kg (OECD Test Guideline 402)

**Skin corrosion/irritation**

Skin - Rabbit

Result: slight irritation - 72 h (OECD Test Guideline 404)

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: slight irritation (OECD Test Guideline 405)

**Respiratory or skin sensitization**

(OECD Test Guideline 406)

**Germ cell mutagenicity**

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 471

Result: negative

Test Type: Mutagenicity (mammal cell test): chromosome aberration. Test system: Human lymphocytes

Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 473

Result: negative

Test Type: In vitro mammalian cell gene mutation test Test system: Mouse lymphoma test

Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 476

Result: negative

**Carcinogenicity**

No data available

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Toxicity**

LD50 orally in Rabbit: 2000 - 2450 mg/kg

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## SECTION 12: Ecological information

**Toxicity****Toxicity to fish**

semi-static test LC50 - Oryzias latipes (Orange-red killifish) - 0,326 mg/l - 96 h

(OECD Test Guideline 203)

#### **Toxicity to daphnia and other aquatic invertebrates**

semi-static test EC50 - *Daphnia magna* (Water flea) - 0,0243 mg/l - 48 h  
(OECD Test Guideline 202)

semi-static test NOEC - *Daphnia magna* (Water flea) - 0,0037 mg/l - 48 h  
(OECD Test Guideline 202)

#### **Toxicity to algae**

semi-static test EC50 - *Pseudokirchneriella subcapitata* (green algae)  
- 0,033 mg/l - 72 h (OECD Test Guideline 201)

semi-static test NOEC - *Pseudokirchneriella subcapitata* (green algae)  
- 0,0038 mg/l - 72 h (OECD Test Guideline 201)

#### **Persistence and degradability**

Biodegradability Result: 10 % - Not readily biodegradable.  
(OECD Test Guideline 301D)

#### **Bioaccumulative potential**

No data available

#### **Mobility in soil**

No data available

#### **Results of PBT and vPvB assessment**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

#### **Other adverse effects**

Very toxic to aquatic life with long lasting effects. Very toxic to aquatic life with long lasting effects.

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## **SECTION 13: Disposal considerations**

#### **Waste treatment methods**

##### **Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

##### **Contaminated packaging**

Dispose of as unused product.

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## **SECTION 14: Transport information**



### UN number

ADR/RID: 3082 IMDG: 3082 IATA: 3334

### UN proper shipping name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (Octane-1-thiol) IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (Octane-1-thiol)

IATA: Aviation regulated liquid, n.o.s. (Octane-1-thiol)

### Transport hazard class(es)

ADR/RID: 9 IMDG: 9 IATA: 9

### Packaging group

ADR/RID: III IMDG: III IATA: III

### Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

### Special precautions for user

### Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

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## SECTION 15: Regulatory information

### Safety, health and environmental regulations/legislation specific for the substance or mixture

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015: Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory: Listed. website: <https://chemicaldata.gov.vn/>

EC Inventory: Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS): Listed. website: <https://echa.europa.eu/>

United States Toxic Substances Control Act (TSCA) Inventory: Listed. website: <https://www.epa.gov/>

Korea Existing Chemicals List (KECL): Listed. website: <http://ncis.nier.go.kr>

New Zealand Inventory of Chemicals (NZIoC): Listed. website: <https://www.epa.govt.nz/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC): Listed. website: <https://www.mee.gov.cn/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS): Listed. website: <https://emb.gov.ph/>

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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  
Chemical Book

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

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 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)
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.