

SAFETY DATA SHEETS

According to Globally Harmonized System of Classification and Labelling of Chemicals (GHS) - Sixth revised edition

Version: 1.0

Creation Date: Aug 10, 2017

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1. Identification

1.1 GHS Product identifier

Product name 1-Mercaptooctane

1.2 Other means of identification

Product number -

Other names n-Octyl Mercaptan

1.3 Recommended use of the chemical and restrictions on use

Identified uses For industry use only. Intermediates, Process regulators

Uses advised against no data available

2. Hazard identification

2.1 Classification of the substance or mixture

Skin sensitization, Category 1

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

2.2 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.

P273 Avoid release to the environment.

Response

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

P333+P313 If skin irritation or rash occurs: Get medical advice/attention.

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 ...

2.3 Other hazards which do not result in classification

none

3. Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
1-Mercaptooctane	1-Mercaptooctane	111-88-6	none	100%

4. First-aid measures

4.1 Description of necessary first-aid measures

General advice

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

If inhaled

Fresh air, rest. Refer for medical attention.

In case of skin contact

Rinse and then wash skin with water and soap.

In case of eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

If swallowed

Rinse mouth. Refer for medical attention .

4.2 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)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

/SRP:/ 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/

5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media

Alcohol foam.

5.2 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)

5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

6.2 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.

6.3 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.

7. Handling and storage

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Avoid exposure - obtain special instructions before use. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

7.2 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.

8. Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

Recommended Exposure Limit: 15 Min Ceiling Value: 0.5 ppm (3.0 mg/cu m).

Biological limit values

no data available

8.2 Appropriate engineering controls

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

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Safety glasses with side-shields conforming to EN166. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Wear impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the

specific workplace. 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 EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

Wear dust mask when handling large quantities.

Thermal hazards

no data available

9. Physical and chemical properties

Physical state	clear liquid
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 37.78°C and below 60°C.Combustible. Gives off irritating or toxic fumes (or gases) in a fire.
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 value)	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

10. Stability and reactivity

10.1 Reactivity

no data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

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

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

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

10.6 Hazardous decomposition products

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

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

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

12. Ecological information

12.1 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

12.2 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).

12.3 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).

12.4 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.

12.5 Other adverse effects

no data available

13. Disposal considerations

13.1 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.

14. Transport information

14.1 UN Number

ADR/RID: UN3082

IMDG: UN3082

IATA: UN3082

14.2 UN Proper Shipping Name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.

IATA: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.

14.3 Transport hazard class(es)

ADR/RID: 9

IMDG: 9

IATA: 9

14.4 Packing group, if applicable

ADR/RID: III

IMDG: III

IATA: III

14.5 Environmental hazards

ADR/RID: yes

IMDG: yes

IATA: yes

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

no data available

15. Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
1-Mercaptooctane	1-Mercaptooctane	111-88-6	none
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.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Not Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.

16. Other information

Information on revision

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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
- 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: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any damage resulting from handling or from contact with the above product.