

## SAFETY DATA SHEET

Version 8.3  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 1-Hexanethiol

Product Number : 739286  
Brand : Aldrich  
CAS-No. : 111-31-9

**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226  
Acute toxicity, Oral (Category 4), H302

For the full text of the H-Statements mentioned in this Section, see Section 16.

**2.2 GHS Label elements, including precautionary statements**

Pictogram



Signal word

Warning

Hazard statement(s)

H226

Flammable liquid and vapor.

H302

Harmful if swallowed.

|                            |                                                                                                      |
|----------------------------|------------------------------------------------------------------------------------------------------|
| Precautionary statement(s) |                                                                                                      |
| P210                       | Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.                                  |
| P233                       | Keep container tightly closed.                                                                       |
| P240                       | Ground/bond container and receiving equipment.                                                       |
| P241                       | Use explosion-proof electrical/ ventilating/ lighting/ equipment.                                    |
| P242                       | Use only non-sparking tools.                                                                         |
| P243                       | Take precautionary measures against static discharge.                                                |
| P264                       | Wash skin thoroughly after handling.                                                                 |
| P270                       | Do not eat, drink or smoke when using this product.                                                  |
| P280                       | Wear protective gloves/ eye protection/ face protection.                                             |
| P301 + P312 + P330         | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.                          |
| P303 + P361 + P353         | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower. |
| P370 + P378                | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.                 |
| P403 + P235                | Store in a well-ventilated place. Keep cool.                                                         |
| P501                       | Dispose of contents/ container to an approved waste disposal plant.                                  |

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Stench.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : 1-Mercaptohexane  
MCH

Formula : C<sub>6</sub>H<sub>14</sub>S  
Molecular weight : 118.24 g/mol  
CAS-No. : 111-31-9  
EC-No. : 203-857-0

| Component             | Classification                            | Concentration |
|-----------------------|-------------------------------------------|---------------|
| <b>Hexane-1-thiol</b> |                                           |               |
|                       | Flam. Liq. 3; Acute Tox. 4;<br>H226, H302 | <= 100 %      |

For the full text of the H-Statements mentioned in this Section, see Section 16.

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

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

#### If inhaled

After inhalation: fresh air.

**In case of skin contact**

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

**In case of eye contact**

After eye contact: rinse out with plenty of water. Remove contact lenses.

**If swallowed**

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

**4.2 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

**4.3 Indication of any immediate medical attention and special treatment needed**

No data available

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**SECTION 5: Firefighting measures****5.1 Extinguishing media****Unsuitable extinguishing media**

For this substance/mixture no limitations of extinguishing agents are given.

**5.2 Special hazards arising from the substance or mixture**

Carbon oxides

Sulfur oxides

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

**5.3 Advice for firefighters**

In the event of fire, wear self-contained breathing apparatus.

**5.4 Further information**

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

**6.2 Environmental precautions**

Do not let product enter drains. Risk of explosion.

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

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemisorb® ). Dispose of properly. Clean up affected area.

**6.4 Reference to other sections**

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

#### Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

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

#### Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Handle under nitrogen, protect from moisture. Store under nitrogen.

#### Storage class

Storage class (TRGS 510): 3: Flammable liquids

### 7.3 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

### 8.1 Control parameters

#### Ingredients with workplace control parameters

| Component      | CAS-No.  | Value | Control parameters               | Basis                                  |
|----------------|----------|-------|----------------------------------|----------------------------------------|
| Hexane-1-thiol | 111-31-9 | C     | 0.5 ppm<br>2.7 mg/m <sup>3</sup> | USA. NIOSH Recommended Exposure Limits |

### 8.2 Exposure controls

#### Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

#### Personal protective equipment

##### Eye/face protection

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

##### Skin protection

required

##### Body Protection

Flame retardant antistatic protective clothing.

##### Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

### **Control of environmental exposure**

Do not let product enter drains. Risk of explosion.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

|                                                 |                                                           |
|-------------------------------------------------|-----------------------------------------------------------|
| a) Appearance                                   | Form: clear, liquid<br>Color: colorless                   |
| b) Odor                                         | Stench.                                                   |
| c) Odor Threshold                               | No data available                                         |
| d) pH                                           | No data available                                         |
| e) Melting point/freezing point                 | Melting point/range: -81 - -80 °C (-114 - -112 °F) - lit. |
| f) Initial boiling point and boiling range      | 150 - 154 °C 302 - 309 °F - lit.                          |
| g) Flash point                                  | 38.9 °C (102.0 °F)                                        |
| h) Evaporation rate                             | No data available                                         |
| i) Flammability (solid, gas)                    | No data available                                         |
| j) Upper/lower flammability or explosive limits | No data available                                         |
| k) Vapor pressure                               | No data available                                         |
| l) Vapor density                                | No data available                                         |
| m) Density                                      | 0.832 g/cm <sup>3</sup> at 25 °C (77 °F)                  |
| Relative density                                | No data available                                         |
| n) Water solubility                             | No data available                                         |
| o) Partition coefficient: n-octanol/water       | No data available                                         |
| p) Autoignition temperature                     | No data available                                         |
| q) Decomposition temperature                    | No data available                                         |
| r) Viscosity                                    | No data available                                         |
| s) Explosive properties                         | No data available                                         |
| t) Oxidizing properties                         | none                                                      |

### **9.2 Other safety information**

No data available

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## **SECTION 10: Stability and reactivity**

### **10.1 Reactivity**

Vapor/air-mixtures are explosive at intense warming.

### **10.2 Chemical stability**

The product is chemically stable under standard ambient conditions (room temperature) .

### **10.3 Possibility of hazardous reactions**

No data available

### **10.4 Conditions to avoid**

Heating.

### **10.5 Incompatible materials**

Bases, Oxidizing agents, Reducing agents, Alkali metals

### **10.6 Hazardous decomposition products**

In the event of fire: see section 5

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## **SECTION 11: Toxicological information**

### **11.1 Information on toxicological effects**

#### **Acute toxicity**

LD50 Oral - Rat - 1,254 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity).

Respiratory disorder

Behavioral:Coma.

Inhalation: No data available

Dermal: No data available

No data available

#### **Skin corrosion/irritation**

No data available

#### **Serious eye damage/eye irritation**

No data available

#### **Respiratory or skin sensitization**

No data available

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

#### **Reproductive toxicity**

No data available

No data available

#### **Specific target organ toxicity - single exposure**

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No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

Nausea, Headache, Vomiting

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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**SECTION 12: Ecological information**

**12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

No data available

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Other adverse effects**

No data available

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**SECTION 13: Disposal considerations**

**13.1 Waste treatment methods**

**Product**

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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**SECTION 14: Transport information**

**DOT (US)**

UN number: 1228    Class: 3 (6.1)    Packing group: III  
Proper shipping name: Mercaptans, liquid, flammable, toxic, n.o.s.  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

**IMDG**

UN number: 1228    Class: 3 (6.1)    Packing group: III    EMS-No: F-E, S-D

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Proper shipping name: MERCAPTANS, LIQUID, FLAMMABLE, TOXIC, N.O.S. (Hexane-1-thiol)

**IATA**

UN number: 1228 Class: 3 (6.1)

Packing group: III

Proper shipping name: Mercaptans, liquid, flammable, toxic, n.o.s. (Hexane-1-thiol)

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**SECTION 15: Regulatory information**

**SARA 302 Components**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 313 Components**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**

Fire Hazard, Acute Health Hazard

**Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

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**SECTION 16: Other information**

**Further information**

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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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