

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : 1-Hexanethiol

Product Number : 234192  
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  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

#### 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

### 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 vapour.  
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.

P303 + P361 + P353 Rinse mouth.  
 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.

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**3. COMPOSITION/INFORMATION ON INGREDIENTS**

**3.1 Substances**

Synonyms : Hexyl mercaptan  
 Mercaptan C6

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

**Hazardous components**

Component	Classification	Concentration
<b>Hexane-1-thiol</b>		
	Flam. Liq. 3; Acute Tox. 4; H226, H302	90 - 100 %

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

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**4. FIRST AID MEASURES**

**4.1 Description of first aid measures**

**General advice**

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

**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.

**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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**5. FIREFIGHTING MEASURES**

**5.1 Extinguishing media**

**Suitable extinguishing media**

Dry powder Dry sand

**Unsuitable extinguishing media**

Do NOT use water jet.

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

No data available

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

Use water spray to cool unopened containers.

**6. ACCIDENTAL RELEASE MEASURES****6.1 Personal precautions, protective equipment and emergency procedures**

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

For personal protection see section 8.

**6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

**6.3 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).

**6.4 Reference to other sections**

For disposal see section 13.

**7. HANDLING AND STORAGE****7.1 Precautions for safe handling**

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

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

For precautions see section 2.2.

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

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.

**7.3 Specific end use(s)**

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

**8. EXPOSURE CONTROLS/PERSONAL PROTECTION****8.1 Control parameters****Components with workplace control parameters**

Component	CAS-No.	Value	Control parameters	Basis
Hexane-1-thiol	111-31-9	C	0.500000 ppm 2.700000 mg/m3	USA. NIOSH Recommended Exposure Limits
	Remarks	15 minute ceiling value		

**8.2 Exposure controls****Appropriate engineering controls**

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

**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.

**Body Protection**

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., 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.

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**9. PHYSICAL AND CHEMICAL PROPERTIES****9.1 Information on basic physical and chemical properties**

a) Appearance	Form: clear, liquid Colour: colourless
b) Odour	Stench.
c) Odour 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	30 °C (86 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapour pressure	No data available
l) Vapour density	No data available
m) Relative density	0.838 g/cm <sup>3</sup> at 25 °C (77 °F)
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Auto-ignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

**9.2 Other safety information**

No data available

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## 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

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Bases, Oxidizing agents, Reducing agents, Alkali metals

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulphur oxides

Other decomposition products - No data available

In the event of fire: see section 5

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## 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 sensitisation

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

IARC: No component 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 component 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 identified as a carcinogen or potential carcinogen by OSHA.

#### Reproductive toxicity

No data available

No data available

#### Specific target organ toxicity - single exposure

No data available

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

No data available

**Additional Information**

RTECS: MO4550000

Nausea, Headache, Vomiting

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

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**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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**13. DISPOSAL CONSIDERATIONS****13.1 Waste treatment methods****Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**

Dispose of as unused product.

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**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

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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**15. REGULATORY INFORMATION****SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**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.

### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Hexane-1-thiol	111-31-9	2007-03-01

	CAS-No.	Revision Date
Hexane-1-thiol	111-31-9	2007-03-01

### New Jersey Right To Know Components

	CAS-No.	Revision Date
Hexane-1-thiol	111-31-9	2007-03-01

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Flam. Liq.	Flammable liquids
H226	Flammable liquid and vapour.
H302	Harmful if swallowed.

### HMIS Rating

Health hazard:	1
Chronic Health Hazard:	
Flammability:	3
Physical Hazard	0

### NFPA Rating

Health hazard:	1
Fire Hazard:	3
Reactivity Hazard:	0

### Further information

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### Preparation Information

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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