

Chemical Safety Data Sheet MSDS / SDS

1-Hexanethiol

Revision Date:2023-12-02 Revision Number:1

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

Product identifier

Product name : 1-Hexanethiol
CBnumber : CB9852837
CAS : 111-31-9
EINECS Number : 203-857-0
Synonyms : 1-hexanethiol,hexanethiol

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 : 400-158-6606

SECTION 2: Hazards identification

Classification of the substance or mixture

Flammable liquids, Category 2
Acute toxicity - Category 4, Dermal
Acute toxicity - Category 4, Inhalation

Label elements**Pictogram(s)**

☐☐☐

Signal word : Warning

Hazard statement(s)

H226 Flammable liquid and vapour
H302 Harmful if swallowed
H331 Toxic if inhaled

Precautionary statement(s)

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P309 IF exposed or if you feel unwell:

P310 Immediately call a POISON CENTER or doctor/physician.

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

P403 Store in a well-ventilated place.

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P233 Keep container tightly closed.

P240 Ground and bond container and receiving equipment.

P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.

P242 Use non-sparking tools.

P243 Take action to prevent static discharges.

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

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].

P370+P378 In case of fire: Use ... to extinguish.

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

P317 Get medical help.

P321 Specific treatment (see ... on this label).

P362+P364 Take off contaminated clothing and wash it before reuse.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.

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

no data available

SECTION 3: Composition/information on ingredients

Substance

| | |
|--------------|-----------------------------|
| Product name | : 1-Hexanethiol |
| Synonyms | : 1-hexanethiol,hexanethiol |
| CAS | : 111-31-9 |
| EC number | : 203-857-0 |
| MF | : C6H14S |
| MW | : 118.24 |

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

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. Give one or two glasses of water to drink. Do NOT induce vomiting. Refer for medical attention .

Most important symptoms and effects, both acute and delayed

Exposure Routes: inhalation, ingestion, skin and/or eye contact Symptoms: Irritation eyes, skin, nose, throat; lassitude (weakness, exhaustion), cyanosis, increased respiration, nausea, drowsiness, headache, vomiting Target Organs: Eyes, skin, respiratory system, central nervous system, blood (NIOSH, 2016)

Indication of any immediate medical attention and special treatment needed

no data available

SECTION 5: Firefighting measures

Extinguishing media

Excerpt from ERG Guide 131 [Flammable Liquids - Toxic]: CAUTION: All these products have a very low flash point: Use of water spray when fighting fire may be inefficient. SMALL FIRE: Dry chemical, CO₂, water spray or alcohol-resistant foam. LARGE FIRE: Water spray, fog or alcohol-resistant foam. Move containers from fire area if you can do it without risk. Dike fire-control water for later disposal; do not scatter the material. Use water spray or fog; do not use straight streams. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. For massive fire, use unmanned hose holders or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2016)

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)

Advice for firefighters

Use water spray, powder, alcohol-resistant foam, carbon dioxide.

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 3 Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions. Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, [acetone](#))

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N₂](#))

SPEC.

HAZ.

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. Remove all ignition sources. Cover the spilled material with inert absorbent. Sweep spilled substance into covered sealable containers. Do NOT wash away into sewer.

Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Remove all ignition sources. Cover the spilled material with inert absorbent. Sweep spilled substance into covered sealable containers. Do NOT wash away into sewer.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. 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.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

| | | | | |
|-------------|---------------------------|-------------------|--------------------------|-------------------|
| Component | Hexane-1-thiol | | | |
| CAS No. | 111-31-9 | | | |
| | Limit value - Eight hours | | Limit value - Short term | |
| | ppm | mg/m ³ | ppm | mg/m ³ |
| USA - NIOSH | ? | ? | 0,5 (1) | 2,7 (1) |
| | Remarks | | | |
| USA - NIOSH | (1) Ceiling limit value | | | |

Biological limit values

no data available

Exposure 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

Eye/face protection

Wear safety spectacles or eye protection in combination with breathing protection.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

| | |
|--|--|
| Physical state | Liquid |
| Colour | Clear colorless to yellow |
| Odour | no data available |
| Melting point/freezing point | -81°C(lit.) |
| Boiling point or initial boiling point and boiling range | 150°C |
| Flammability | Class IB Flammable Liquid: F.I.P. below 73°F and BP at or above 100°F. |
| Lower and upper explosion limit/flammability limit | no data available |
| Flash point | 30°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 | 5.35 |
| Vapour pressure | 4.5mmHg at 25°C |
| Density and/or relative density | 0.842 (20/4°C) |
| Relative vapour density | 0.842 (20/4°C) |
| Particle characteristics | no data available |

SECTION 10: Stability and reactivity

Reactivity

Reacts with acids, bases and strong oxidants. Decomposes on burning. This produces toxic and corrosive fumes including hydrogen sulfide and sulfur oxides.

Chemical stability

no data available

Possibility of hazardous reactions

The vapour is heavier than air and may travel along the ground; distant ignition possible. n-HEXANETHIOL is incompatible with oxidizing agents, strong acids and strong bases, alkali metals, and nitric acid. Can react with water, steam or acids to produce toxic and flammable vapors. Reacts violently with powerful oxidizing agents such as calcium hypochlorite ($\text{Ca}(\text{OCl})_2$) to generate SO_x . Reacts with hydrides to form flammable H_2 gas; reacts with halogenated hydrocarbons to yield HX . Reacts exothermically with aldehydes. Emits toxic compounds of sulfur when heated to decomposition.

Conditions to avoid

no data available

Incompatible materials

Oxidizers, reducing agents, strong acids & bases, alkali metals

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- 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 irritating to the eyes, skin and respiratory tract. The substance may cause effects on the central nervous system. This may result in 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

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

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: UN1228 (For reference only, please check.)

IMDG: UN1228 (For reference only, please check.)

IATA: UN1228 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: MERCAPTANS, LIQUID, FLAMMABLE, TOXIC, N.O.S. or MERCAPTAN MIXTURE, LIQUID, FLAMMABLE, TOXIC, N.O.S. (For reference only, please check.)

IMDG: MERCAPTANS, LIQUID, FLAMMABLE, TOXIC, N.O.S. or MERCAPTAN MIXTURE, LIQUID, FLAMMABLE, TOXIC, N.O.S. (For reference only, please check.)

IATA: MERCAPTANS, LIQUID, FLAMMABLE, TOXIC, N.O.S. or MERCAPTAN MIXTURE, LIQUID, FLAMMABLE, TOXIC, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)

IMDG: 3 (For reference only, please check.)

IATA: 3 (For reference only, please check.)

Packing group, if applicable

ADR/RID: II (For reference only, please check.)

IMDG: II (For reference only, please check.)

IATA: II (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

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

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/>

Other Information

Health effects of exposure to the substance have not been investigated adequately.

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.