

Chemical Safety Data Sheet MSDS / SDS

Hexadecane-1-thiol SDS

Revision Date:2024-04-25 Revision Number:1

Section 1	Section 2	Section 3	Section 4	Section 5	Section 6	Section 7	Section 8
Section 9	Section 10	Section 11	Section 12	Section 13	Section 14	Section 15	Section 16

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

Product name: Hexadecane-1-thiol
CAS: 2917-26-2

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.in
Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090
Telephone: +91 9550333722

SECTION 2: Hazards identification**Classification of the substance or mixture**

Eye irritation, Category 2
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 4

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H319 Causes serious eye irritation

H413 May cause long lasting harmful effects to aquatic life

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

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

P273 Avoid release to the environment.

Response

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

Storage

none

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 which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	Hexadecane-1-thiol
Common names and synonyms:	Hexadecane-1-thiol
CAS number:	2917-26-2
EC number:	220-846-6
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

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.

Most important symptoms/effects, acute and delayed

Exposure Routes: inhalation, skin absorption, ingestion, skin and/or eye contact Symptoms: Irritation eyes, skin, respiratory system; headache, dizziness, lassitude (weakness, exhaustion), cyanosis, nausea, convulsions Target Organs: Eyes, skin, respiratory system, central nervous system, blood (NIOSH, 2016)

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

no data available

SECTION 5: Firefighting measures

Suitable 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)

Special protective actions for fire-fighters

Use foam, carbon dioxide, powder.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Carefully collect remainder. Then store and dispose of according to local regulations.

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. 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

Separated from strong oxidants, reducing agents, metals and acids.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	Hexadecane-1-thiol			
CAS No.	2917-26-2			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m ³	ppm	mg/m ³
USA - NIOSH	?	?	0,5 (1)	5,3 (1)
	Remarks			
USA - NIOSH	(1) Ceiling limit value (15 min)			

Biological limit values

no data available

Appropriate engineering 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, such as personal protective equipment (PPE)

Eye/face protection

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

Skin protection

Protective gloves.

Respiratory protection

Use ventilation.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	1-hexadecanethiol is a colorless liquid or white solid (below 19° C) with a strong unpleasant odor. Density (as liquid at 25°C): 0.83 g/cm ³ .
Colour:	no data available
Odour:	no data available
Melting point/freezing point:	18-20°C
Boiling point or initial boiling point and boiling range:	184-191°C/7mmHg(lit.)
Flammability:	Class IIIB Combustible Liquid: Fl.P. at or above 200°F.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	102°C
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:	no data available
Vapour pressure:	0.000237mmHg at 25°C
Density and/or relative density:	0.84g/mL at 25°C (lit.)
Relative vapour density:	(air = 1): 8.9
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. This produces toxic gases including sulfur oxides. Reacts violently with strong oxidants, acids, reducing agents and metals.

Chemical stability

no data available

Possibility of hazardous reactions

1-HEXADECANETHIOL Class IIIB is non-flammable but combustible (flash point exceeds 200°F). 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 hydrogen halides. Reacts exothermically with aldehydes. Emits toxic compounds of sulfur when heated to decomposition.

Conditions to avoid

no data available

Incompatible materials

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

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 mildly irritating to the eyes, skin and respiratory tract.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance 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: UN3334 (For reference only, please check.)

IMDG: UN3334 (For reference only, please check.)

IATA: UN3334 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: AVIATION REGULATED LIQUID, N.O.S. (For reference only, please check.)

IMDG: AVIATION REGULATED LIQUID, N.O.S. (For reference only, please check.)

IATA: AVIATION REGULATED LIQUID, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 9 (For reference only, please check.)

IMDG: 9 (For reference only, please check.)

IATA: 9 (For reference only, please check.)

Packing group, if applicable

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

IMDG: (For reference only, please check.)

IATA: (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

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Not Listed.

Korea Existing Chemicals List (KECL)

Not 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

The auto-ignition temperature is unknown in the literature. Health effects of exposure to the substance have not been investigated adequately.

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