

Chemical Safety Data Sheet MSDS / SDS

Pentane-1-thiol SDS

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

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

Product name: Pentane-1-thiol
CAS: 110-66-7

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**

Acute toxicity - Category 4, Oral
Acute toxicity - Category 4, Inhalation

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H302 Harmful if swallowed

H332 Harmful if inhaled

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

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

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

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

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

P317 Get medical help.

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:	Pentane-1-thiol
Common names and synonyms:	Pentane-1-thiol
CAS number:	110-66-7
EC number:	203-789-1
Concentration:	100%

SECTION 4: First aid measures

Description of necessary 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/effects, acute and delayed

Inhalation may cause nausea because of offensive odor. Contact with eyes or skin causes slight irritation. Ingestion may cause vomiting. (USCG, 1999)

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

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

SECTION 5: Firefighting measures

Suitable extinguishing media

Foam, carbon dioxide, dry chemical.

Specific hazards arising from the chemical

Special Hazards of Combustion Products: Sulfur dioxide gas is formed Behavior in Fire: Vapor is heavier than air and may travel considerable distance to a source of ignition and flash back. (USCG, 1999)

Special protective actions for fire-fighters

Use powder, AFFF, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

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

Spills of thiols can be neutralized with a household bleach solution and flushed with an abundant flow of water. Thiols

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Closed system, ventilation, explosion-proof electrical equipment and lighting. 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. Protect containers from physical damage. Store in cool and well-ventilated places, and separate from strong oxidizing materials. Outdoor or detached storage is preferred. For indoor storage, standard combustible liquid room is recommendable.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	Pentane-1-thiol			
CAS No.	110-66-7			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m ³	ppm	mg/m ³
USA - NIOSH	?	?	0,5 (1)	2,1 (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 spectacles.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Amyl mercaptan is a clear colorless to light-yellow liquid with an offensive odor. Flash point 65°F. Less dense than water and insoluble in water. Hence floats on water. Vapors are heavier than air. May be toxic by inhalation.
Colour:	Liquid
Odour:	STRONG, OFFENSIVE
Melting point/freezing point:	198°C(lit.)
Boiling point or initial boiling point and boiling range:	126°C
Flammability:	Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	18°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 Kow = 2.74 (est)
Vapour pressure:	27.4 mm Hg (37.7 °C)
Density and/or relative density:	0.84
Relative vapour density:	3.59 (Air= 1)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

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

Chemical stability

no data available

Possibility of hazardous reactions

Flammable, dangerous fire risk. /Mixture of isomers/The vapour mixes well with air, explosive mixtures are easily formed. AMYL MERCAPTAN is incompatible with oxidizing agents, reducing agents, alkali metals, calcium hypochlorite, concentrated nitric acid (NIOSH, 2016).

Conditions to avoid

no data available

Incompatible materials

Can react vigorously with oxidizing materials.

Hazardous decomposition products

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

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.

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

AEROBIC: n-Amyl mercaptan, present at 500 mg/L, resulted in 375 mg/L O₂ uptake in 168 hours using an activated sludge microbe, *Alcaligenes faecalis*, inoculum at 2,500 bacterial cells/L and the Warburg respirometer test at 20 deg C(1); overall the thiols were not as readily oxidized as were the corresponding alcohols(1). However, pure culture studies such as this are not appropriate for evaluating environmental biodegradation(2).

Bioaccumulative potential

An estimated BCF of 36 was calculated for n-amyl mercaptan(SRC), using a water solubility of 156 mg/L(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, provided the compound is not metabolized by the organism(SRC).

Mobility in soil

The Koc of n-amyl mercaptan is estimated as 270(SRC), using a water solubility of 156 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that n-amyl mercaptan is expected to have

moderate mobility in soil.

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: UN1111 (For reference only, please check.)

IMDG: UN1111 (For reference only, please check.)

IATA: UN1111 (For reference only, please check.)

UN Proper Shipping Name

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

IMDG: AMYL MERCAPTAN (For reference only, please check.)

IATA: AMYL MERCAPTAN (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)

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

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