

Material Safety Data Sheet

Version 3.1

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1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Benzenethiol

Product Number : W361607

Brand : Aldrich

Supplier : Sigma-Aldrich
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USA

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Preparation Information : Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards

Combustible Liquid, Highly toxic by inhalation, Highly toxic by ingestion, Highly toxic by skin absorption, Irritant

Other hazards which do not result in classification

Stench.

GHS Classification

Flammable liquids (Category 3)

Acute toxicity, Oral (Category 2)

Acute toxicity, Inhalation (Category 1)

Acute toxicity, Dermal (Category 2)

Serious eye damage (Category 1)

GHS Label elements, including precautionary statements

Pictogram



Signal word

Danger

Hazard statement(s)

H226

Flammable liquid and vapour.

H300 + H310

Fatal if swallowed or in contact with skin

H318

Causes serious eye damage.

H330

Fatal if inhaled.

Precautionary statement(s)

P260

Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.

P264

Wash hands thoroughly after handling.

P280

Wear protective gloves/ eye protection/ face protection.

P284

Wear respiratory protection.

P302 + P350

IF ON SKIN: Gently wash with plenty of soap and water.

P305 + P351 + P338

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

P310

Immediately call a POISON CENTER or doctor/ physician.

HMIS Classification**Health hazard:** 4**Flammability:** 2**Physical hazards:** 0**NFPA Rating****Health hazard:** 4**Fire:** 2**Reactivity Hazard:** 0**Potential Health Effects****Inhalation** May be fatal if inhaled. Causes respiratory tract irritation.**Skin** May be fatal if absorbed through skin. Causes skin irritation.**Eyes** Causes eye irritation.**Ingestion** May be fatal if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : Phenyl mercaptan
Thiophenol
Benzenethiol

Formula : C₆H₆S
Molecular Weight : 110.18 g/mol

Component		Concentration
Benzenethiol		
CAS-No.	108-98-5	-
EC-No.	203-635-3	

4. 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. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES**Suitable extinguishing media**

For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

Special protective equipment for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products

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

Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

Environmental precautions

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

Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

7. HANDLING AND STORAGE

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.

Conditions for safe storage

Store in cool place. 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.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
Benzenethiol	108-98-5	C	0.1 ppm 0.5 mg/m3	USA. NIOSH Recommended Exposure Limits
Remarks	15 minute ceiling value			
		TWA	0.1 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Upper Respiratory Tract & skin irritation Anemia Danger of cutaneous absorption			
		TWA	0.5 ppm 2 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000

Personal protective equipment

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).

Hand 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.

Eye protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin and 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.

Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	clear, liquid
Colour	colourless

Safety data

pH	no data available
Melting point/freezing point	Melting point/range: -15 °C (5 °F) - lit.
Boiling point	169 °C (336 °F) - lit.
Flash point	50 °C (122 °F) - closed cup
Ignition temperature	450 °C (842 °F)
Autoignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	4.5 hPa (3.4 mmHg) at 40 °C (104 °F) 1.9 hPa (1.4 mmHg) at 20 °C (68 °F)
Density	1.073 g/cm ³ at 25 °C (77 °F)
Water solubility	no data available
Partition coefficient: n-octanol/water	no data available
Relative vapour density	3.8 - (Air = 1.0)
Odour	Stench.
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

no data available

Conditions to avoid

Heat, flames and sparks.

Materials to avoid

Do not store near acids., Strong bases, Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulphur oxides
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50

LD50 Oral - rat - 46.2 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity). Behavioral:Coma. Respiratory disorder

Inhalation LC50

LC50 Inhalation - rat - 4 h - 33 ppm

Remarks: Lungs, Thorax, or Respiration:Respiratory stimulation. Behavioral:Somnolence (general depressed activity). Sense Organs and Special Senses (Nose, Eye, Ear, and Taste):Eye:Lacrimation.

Dermal LD50

LD50 Dermal - rabbit - 134 mg/kg

Remarks: Behavioral:Muscle weakness. Behavioral:Ataxia. Cyanosis

Other information on acute toxicity

no data available

Skin corrosion/irritation**Serious eye damage/eye irritation**

Eyes - rabbit - Severe eye irritation

Respiratory or skin sensitization

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.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

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

Reproductive toxicity - rat - Oral

Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants). Effects on Fertility: Litter size (e.g.; # fetuses per litter; measured before birth). Effects on Embryo or Fetus: Other effects to embryo.

Reproductive toxicity - rat - Oral

Maternal Effects: Other effects.

no data available

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)

no data available

Specific target organ toxicity - repeated exposure (Globally Harmonized System)

no data available

Aspiration hazard

no data available

Potential health effects

Inhalation	May be fatal if inhaled. Causes respiratory tract irritation.
Ingestion	May be fatal if swallowed.
Skin	May be fatal if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.

Signs and Symptoms of Exposure

Cough, Shortness of breath, Headache, Nausea, Vomiting

Synergistic effects

no data available

Additional Information

RTECS: DC0525000

12. ECOLOGICAL INFORMATION

Toxicity

no data available

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

PBT and vPvB assessment

no data available

Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

Product

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

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 2337 Class: 6.1 (3) Packing group: I

Proper shipping name: Phenyl mercaptan

Reportable Quantity (RQ): 100 lbs

Marine pollutant: No

Poison Inhalation Hazard: Hazard zone B

IMDG

UN number: 2337 Class: 6.1 (3) Packing group: I

EMS-No: F-E, S-D

Proper shipping name: PHENYL MERCAPTAN

Marine pollutant: No

IATA

UN number: 2337 Class: 6.1 (3)

Proper shipping name: Phenyl mercaptan

IATA Passenger: Not permitted for transport

IATA Cargo: Not permitted for transport

15. REGULATORY INFORMATION

OSHA Hazards

Combustible Liquid, Highly toxic by inhalation, Highly toxic by ingestion, Highly toxic by skin absorption, Irritant

SARA 302 Components

The following components are subject to reporting levels established by SARA Title III, Section 302:

CAS-No.

Revision Date

SARA 313 Components

SARA 313: 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

Benzenethiol	CAS-No. 108-98-5	Revision Date 2007-07-01
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Pennsylvania Right To Know Components

Benzenethiol	CAS-No. 108-98-5	Revision Date 2007-07-01
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New Jersey Right To Know Components

Benzenethiol	CAS-No. 108-98-5	Revision Date 2007-07-01
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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.

16. OTHER INFORMATION**Further information**

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