



SAFETY DATA SHEET

1. Identification

Product identifier	Benzyl Mercaptan	
Other means of identification		
Catalog number	1062074	
CAS number	100-53-8	
Synonyms	alpha-Toluenethiol	
Chemical name	Benzenemethanethiol	
Recommended use	For analytical laboratory use only.	
Recommended restrictions	Not for use as a drug. Not for administration to humans or animals.	
Manufacturer/Importer/Supplier/Distributor information		
Manufacturer		
Company name	U. S. Pharmacopeia	
Address	12601 Twinbrook Parkway Rockville MD 20852-1790 United States	
Telephone	Customer Service	301-881-0666
Website	www.usp.org	
E-mail	RSTECH@usp.org	
Emergency phone number	CHEMTREC within US & Canada	1-800-424-9300
	CHEMTREC outside US & Canada	+1 703-527-3887

2. Hazard(s) identification

Physical hazards	Flammable liquids	Category 4
Health hazards	Acute toxicity, oral	Category 4
	Acute toxicity, inhalation	Category 2
	Serious eye damage/eye irritation	Category 2A
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	
Label elements		



Signal word	Danger
Hazard statement	Combustible liquid. Harmful if swallowed. Fatal if inhaled. Causes serious eye irritation.
Precautionary statement	
Prevention	Keep away from flames and hot surfaces. - No smoking. Wear protective gloves/eye protection/face protection. Wash thoroughly after handling. Do not breathe dust/fume/gas/mist/vapors/spray. Use only outdoors or in a well-ventilated area. In case of inadequate ventilation wear respiratory protection.
Response	In case of fire: Use appropriate media to extinguish. If swallowed: Call a poison center/doctor if you feel unwell. Rinse mouth. If inhaled: Remove person to fresh air and keep comfortable for breathing. Immediately call a poison center/doctor. If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
Storage	Store in a well-ventilated place. Keep cool. Keep container tightly closed. Store locked up.

Disposal	Dispose of contents/container in accordance with local/regional/national/international regulations.
Hazard(s) not otherwise classified (HNOC)	None known.
Supplemental information	None.

3. Composition/information on ingredients

Substance

Chemical name	Common name and synonyms	CAS number	%
Benzyl Mercaptan	alpha-Toluenethiol	100-53-8	100

Information provided in the SDS is not specific to the lot provided. Refer to the label and USP Certificate/Product Information Sheet for the assigned value of a particular lot.

4. First-aid measures

Inhalation	Move to fresh air. Oxygen or artificial respiration if needed. Do not use mouth-to-mouth method if the substance is inhaled. Induce artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Call a physician or poison control center immediately.
Skin contact	Rinse skin with water/shower. Get medical attention if irritation develops and persists.
Eye contact	Immediately flush eyes with plenty of water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical attention if irritation develops and persists.
Ingestion	Rinse mouth. Do not induce vomiting without advice from poison control center. If vomiting occurs, keep head low so that stomach content doesn't get into the lungs. Get medical advice/attention if you feel unwell.
Most important symptoms/effects, acute and delayed	Not available.
Indication of immediate medical attention and special treatment needed	Provide general supportive measures and treat symptomatically.
General information	Remove from exposure. Remove contaminated clothing. For treatment advice, seek guidance from an occupational health physician or other licensed health-care provider familiar with workplace chemical exposures. In the United States, the national poison control center phone number is 1-800-222-1222. If person is not breathing, give artificial respiration. If breathing is difficult, give oxygen if available. Persons developing serious hypersensitivity (anaphylactic) reactions must receive immediate medical attention.

5. Fire-fighting measures

Suitable extinguishing media	Water fog. Foam. Dry chemical powder. Carbon dioxide (CO2).
Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.
Specific hazards arising from the chemical	No unusual fire or explosion hazards noted.
Special protective equipment and precautions for firefighters	Wear suitable protective equipment.
General fire hazards	Combustible liquid.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures	Keep unnecessary personnel away. ELIMINATE all ignition sources (no smoking, flares, sparks or flames in immediate area). Wear appropriate personal protective equipment. Avoid inhalation of vapors. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Ensure adequate ventilation. For personal protection, see section 8 of the SDS.
Methods and materials for containment and cleaning up	ELIMINATE all ignition sources (no smoking, flares, sparks or flames in immediate area). Absorb spillage with suitable absorbent material. Keep combustibles (wood, paper, oil, etc.) away from spilled material. For waste disposal, see section 13 of the SDS.
Environmental precautions	Avoid discharge into drains, water courses or onto the ground.

7. Handling and storage

Precautions for safe handling	As a general rule, when handling USP materials, avoid all contact and inhalation of dust, mists, and/or vapors associated with the material. Clean equipment and work surfaces with suitable detergent or solvent after use. After removing gloves, wash hands and other exposed skin thoroughly. Select and use containment devices and personal protective equipment based on a risk assessment of material potency and exposure potential.
Conditions for safe storage, including any incompatibilities	Store in tight container. This material should be handled and stored per label instructions to ensure product integrity.

8. Exposure controls/personal protection

Occupational exposure limits	No exposure limits noted for ingredient(s).
Biological limit values	No biological exposure limits noted for the ingredient(s).
Appropriate engineering controls	For laboratory operations, use good technique and limit open handling. Control exposures to below the occupational exposure level (if available). Select and use containment devices and personal protective equipment based on a risk assessment of exposure potential. Cover all containers for solutions and slurries while being transferred.
Individual protection measures, such as personal protective equipment	
Eye/face protection	Wear safety glasses with side shields, chemical splash goggles, or full face shield, if necessary. Base the choice of protection on the job activity and potential for contact with eyes or face. An emergency eye wash station should be available.
Skin protection	
Hand protection	Consider double gloves. Wear nitrile or other impervious gloves if skin contact is possible. When the material is dissolved or suspended in an organic solvent, wear gloves that provide protection against the solvent.
Other	Train employees in proper gowning and degowning practices. Wear disposable lab coat, disposable sleeve covers and two pair of gloves as appropriate for the task. Base the choice of skin protection on the job activity, potential for skin contact and solvents and reagents in use. Do not wear protective garments in common areas (e.g., cafeterias) or out-of-doors.
Respiratory protection	Use a powered air-purifying respirator (PAPR) with HEPA filters, disposable outerware and head cover for spill cleanup. Respirators are generally not required for laboratory operations. Choose respiratory protection appropriate to the task and the level of existing engineering controls.
Thermal hazards	Wear appropriate thermal protective clothing, when necessary.
General hygiene considerations	When using do not smoke. Keep away from food and drink. Always observe good personal hygiene measures, such as washing after handling the material and before eating, drinking, and/or smoking. Routinely wash work clothing and protective equipment to remove contaminants. Pharmacological effects may be seen with occupational exposure. Handling practices in this SDS are recommendations for laboratory use of USP materials.

9. Physical and chemical properties

Appearance	Appearance descriptions are general information and not specific to any USP lot.
Physical state	Liquid.
Form	Liquid.
Color	Colorless.
Odor	Characteristic odor. Stench.
Odor threshold	0 - 0.04 ppm
pH	Not available.
Melting point/freezing point	-22 °F (-30 °C)
Initial boiling point and boiling range	381.2 - 383 °F (194 - 195 °C)
Flash point	158.0 °F (70.0 °C)
Evaporation rate	Not available.
Flammability (solid, gas)	Not applicable.
Upper/lower flammability or explosive limits	
Flammability limit - lower (%)	Not available.
Flammability limit - upper (%)	Not available.
Explosive limit - lower (%)	Not available.

Explosive limit - upper (%)	Not available.
Vapor pressure	0.06 kPa (77 °F (25 °C))
Vapor density	4.28 (air = 1)
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Insoluble.
Solubility (other)	Ethanol: Very soluble. Ether: Very soluble. Carbon Disulfide: Soluble. Carbon Tetrachloride: Slightly soluble.
Partition coefficient (n-octanol/water)	2.5
Auto-ignition temperature	Not available.
Decomposition temperature	Not available.
Viscosity	Not available.
Other information	
Chemical family	Thiol.
Molecular formula	C7H8S
Molecular weight	124.2
Specific gravity	1.06 at 20 °C

10. Stability and reactivity

Reactivity	The product is stable and non-reactive under normal conditions of use, storage and transport.
Chemical stability	Material is stable under normal conditions.
Possibility of hazardous reactions	No dangerous reaction known under conditions of normal use.
Conditions to avoid	Avoid heat, sparks, open flames and other ignition sources. Contact with incompatible materials. This material oxidizes in air to dibenzyl disulfide, which is a sensitizer.
Incompatible materials	Strong oxidizing agents. Strong bases.
Hazardous decomposition products	Irritating and/or toxic fumes or gases. Emits toxic fumes under fire conditions. SOx.

11. Toxicological information

Information on likely routes of exposure

Inhalation	Fatal if inhaled.
Skin contact	Knowledge about health hazard is incomplete.
Eye contact	Causes serious eye irritation.
Ingestion	Harmful if swallowed.

Symptoms related to the physical, chemical and toxicological characteristics Severe eye irritation. Cough. Shortness of breath. Headache. Nausea. Vomiting. Tearing.

Information on toxicological effects

Acute toxicity Fatal if inhaled. Harmful if swallowed.

Product	Species	Test Results
Benzyl Mercaptan (CAS 100-53-8)		
<u>Acute</u>		
Dermal		
LD50	Rat	> 2000 mg/kg
Inhalation		
LC50	Mouse	178 ppm, 4 Hours
	Rat	> 235 ppm, 4 Hours
Oral		
LD50	Rat	493 mg/kg

Skin corrosion/irritation Based on available data, the classification criteria are not met.
Serious eye damage/eye irritation Causes serious eye irritation.

Local effects

Irritation test (106 mg)
Result: Irritant.
Species: Rabbit
Organ: Eye
Severity: Slight
Irritation test
Result: Non-irritant.
Species: Rabbit
Organ: Skin

Respiratory or skin sensitization

Respiratory sensitization Knowledge about health hazard is incomplete.

Skin sensitization Knowledge about health hazard is incomplete.

Germ cell mutagenicity Knowledge about mutagenicity is incomplete.

Mutagenicity

E. coli
Result: Negative.
S. typhimurium Ames assay
Result: Negative.

Carcinogenicity Knowledge about carcinogenicity is incomplete.

IARC Monographs. Overall Evaluation of Carcinogenicity

Not listed.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)

Not listed.

US. National Toxicology Program (NTP) Report on Carcinogens

Not listed.

Reproductive toxicity Knowledge about health hazard is incomplete.

Specific target organ toxicity - single exposure Knowledge about health hazard is incomplete.

Specific target organ toxicity - repeated exposure Knowledge about health hazard is incomplete.

Aspiration hazard Knowledge about health hazard is incomplete.

12. Ecological information

Ecotoxicity

Product	Species		Test Results
Benzyl Mercaptan (CAS 100-53-8)			
Aquatic			
Acute			
Crustacea	EC50	Daphnia magna	0.15 mg/l, 48 hours

Persistence and degradability Not readily biodegradable.

Bioaccumulative potential

Octanol/water partition coefficient log Kow
2.5

Mobility in soil No data available.

Other adverse effects No other adverse environmental effects (e.g. ozone depletion, photochemical ozone creation potential, endocrine disruption, global warming potential) are expected from this component.

13. Disposal considerations

Disposal instructions Dispose in accordance with all applicable regulations. Under RCRA, it is the responsibility of the user of the product to determine, at the time of disposal, whether the product meets RCRA criteria for hazardous waste.

Local disposal regulations Dispose in accordance with all applicable regulations.

Hazardous waste code	The waste code should be assigned in discussion between the user, the producer and the waste disposal company.
Waste from residues / unused products	Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe manner (see: Disposal instructions).
Contaminated packaging	Since emptied containers may retain product residue, follow label warnings even after container is emptied.

14. Transport information

DOT

UN number	UN2810
UN proper shipping name	Toxic liquid, organic, n.o.s. (Benzyl Mercaptan)
Transport hazard class(es)	
Class	6.1
Subsidiary risk	-
Packing group	II

IATA

UN number	UN2810
UN proper shipping name	Toxic liquid, organic, n.o.s. (Benzyl Mercaptan)
Transport hazard class(es)	
Class	6.1
Subsidiary risk	-
Packing group	II

Other information

Passenger and cargo aircraft Allowed with restrictions.

Cargo aircraft only Allowed with restrictions.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not established.

DOT; IATA



General information It is the shipper's responsibility to determine the correct transport classification at the time of shipment.

15. Regulatory information

US federal regulations This product is a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

Toxic Substances Control Act (TSCA)

TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)

Benzyl Mercaptan (CAS 100-53-8) 1.0 % One-Time Export Notification only.

CERCLA Hazardous Substance List (40 CFR 302.4)

Not listed.

SARA 304 Emergency release notification

Not regulated.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)

Not listed.

Superfund Amendments and Reauthorization Act of 1986 (SARA)

SARA 302 Extremely hazardous substance

Not listed.

SARA 311/312 Hazardous chemical Yes

Classified hazard categories	Flammable (gases, aerosols, liquids, or solids) Acute toxicity (any route of exposure) Serious eye damage or eye irritation
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SARA 313 (TRI reporting)
Not regulated.

Other federal regulations

Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List

Not regulated.

Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)

Not regulated.

Safe Drinking Water Act (SDWA) Not regulated.

FEMA Priority Substances Respiratory Health and Safety in the Flavor Manufacturing Workplace

Benzyl Mercaptan (CAS 100-53-8)	Low priority
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US state regulations

California Proposition 65

California Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65): This material is not known to contain any chemicals currently listed as carcinogens or reproductive toxins. For more information go to www.P65Warnings.ca.gov.

International Inventories

Country(s) or region	Inventory name	On inventory (yes/no)*
Australia	Australian Inventory of Chemical Substances (AICS)	Yes
Canada	Domestic Substances List (DSL)	Yes
Canada	Non-Domestic Substances List (NDSL)	No
China	Inventory of Existing Chemical Substances in China (IECSC)	Yes
Europe	European Inventory of Existing Commercial Chemical Substances (EINECS)	Yes
Europe	European List of Notified Chemical Substances (ELINCS)	No
Japan	Inventory of Existing and New Chemical Substances (ENCS)	Yes
Korea	Existing Chemicals List (ECL)	No
New Zealand	New Zealand Inventory	Yes
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	Yes
Taiwan	Taiwan Chemical Substance Inventory (TCSI)	Yes
United States & Puerto Rico	Toxic Substances Control Act (TSCA) Inventory	Yes

*A "Yes" indicates that all components of this product comply with the inventory requirements administered by the governing country(s)

A "No" indicates that one or more components of the product are not listed or exempt from listing on the inventory administered by the governing country(s).

16. Other information, including date of preparation or last revision

Issue date 10-23-2012

Revision date 12-11-2023

Version # 05

Disclaimer USP materials are sold for analytical laboratory use only, and NOT for human consumption. The information contained herein is applicable solely to the chemical substance when used for analytical laboratory use and does not necessarily relate to any other use of the substance described, (i.e. at different concentrations, in drug dosage forms, or in bulk quantities). USP materials are intended for use by persons having technical skill and at their own discretion and risk. This information has been compiled by USP staff from sources considered to be scientifically reliable but has not been independently verified by USP. USP does not guarantee the accuracy or completeness of the information from these sources included herein nor should the statements contained herein be considered an official expression by USP. USP does not independently create or develop the information included in this safety data sheet. NO REPRESENTATION OR WARRANTY, EXPRESS OR IMPLIED, INCLUDING THE WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE is made with respect to the information contained herein.