SAFETY DATA SHEET

Version 4.10 Revision Date 07/09/2014 Print Date 06/29/2015

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

CAS-No.

Product name : Benzyl mercaptan

Product Number : W214701 Brand : Aldrich

1.2 Relevant identified uses of the substance or mixture and uses advised against

100-53-8

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich

3050 Spruce Street

SAINT LOUIS MO 63103

USA

Telephone : +1 800-325-5832 Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 4), H227 Acute toxicity, Oral (Category 4), H302 Acute toxicity, Inhalation (Category 2), H330

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)

H227 Combustible liquid H302 Harmful if swallowed. H330 Fatal 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.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.

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

protection.

P284 Wear respiratory protection.

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P301 + P312 IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you

feel unwell.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position

comfortable for breathing.

P310 Immediately call a POISON CENTER or doctor/ physician.

P320 Specific treatment is urgent (see supplemental first aid instructions on

this label).

P330 Rinse mouth.

P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for

extinction.

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

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

P405 Store locked up.

P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Stench.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : α-Toluenethiol

α-Tolyl mercaptan

Formula : C₇H₈S

Molecular Weight : 124.20 g/mol
CAS-No. : 100-53-8
EC-No. : 202-862-5

Hazardous components

Component	Classification	Concentration
Toluene-α-thiol		
	Flam. Liq. 4; Acute Tox. 4;	-
	Acute Tox. 2; H227, H302,	
	H330	

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of 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

Flush eyes with water as a precaution.

If swallowed

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

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

no data available

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5. FIREFIGHTING MEASURES

5.1 Extinguishing media

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.

5.2 Special hazards arising from the substance or mixture

Carbon oxides, Sulphur oxides

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, 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.

For personal protection see section 8.

6.2 Environmental precautions

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

6.3 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). Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 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. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

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.

Handle and store under inert gas. Air and moisture sensitive.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

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

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

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Skin 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.

Body Protection

Complete suit protecting against chemicals. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multipurpose 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).

Control of environmental exposure

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

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

Form: clear, liquid Appearance

Colour: colourlesslight yellow

Odour characteristic b)

Odour Threshold no data available c) no data available d) На

Melting point/freezing

point

-30 °C (-22 °F)

Initial boiling point and

194 - 195 °C (381 - 383 °F) - lit.

boiling range

g) Flash point 70 °C (158 °F) - closed cup

Evapouration rate no data available i) Flammability (solid, gas) no data available

Upper/lower flammability or no data available

explosive limits

Vapour pressure 0.625 hPa (0.469 mmHg)

Vapour density 4.29 - (Air = 1.0)

m) Relative density 1.058 g/cm3 at 25 °C (77 °F)

n) Water solubility insoluble

o) Partition coefficient: n-

no data available

octanol/water

no data available

Auto-ignition temperature

no data available

Decomposition temperature

Viscosity no data available r)

Explosive properties no data available s) no data available

Other safety information

9.2

Oxidizing properties

Relative vapour density 4.29 - (Air = 1.0)

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10. STABILITY AND REACTIVITY

10.1 Reactivity

no data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Strong bases, Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - no data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - rat - 493 mg/kg

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

LC50 Inhalation - mouse - 4 h - 178 ppm

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

Dermal: no data available

no data available

Skin corrosion/irritation

no data available

Serious eye damage/eye irritation

no data available

Respiratory or skin sensitisation

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

Carcinogenicity - mouse - Skin

Tumorigenic: Equivocal tumorigenic agent by RTECS criteria. Skin and Appendages: Other: Tumors.

Tumorigenic:Tumors at site or application.

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

no data available

no data available

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Specific target organ toxicity - single exposure

no data available

Specific target organ toxicity - repeated exposure

no data available

Aspiration hazard

no data available

Additional Information

RTECS: XT8650000

Cough, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

no data available

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. 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: 2810 Class: 6.1 Packing group: II Proper shipping name: Toxic, liquids, organic, n.o.s. (Toluene-α-thiol)

Marine pollutant: No

Poison Inhalation Hazard: No

IMDG

UN number: 2810 Class: 6.1 Packing group: II EMS-No: F-A, S-A

Proper shipping name: TOXIC LIQUID, ORGANIC, N.O.S. (Toluene-α-thiol)

Marine pollutant: No

IATA

UN number: 2810 Class: 6.1 Packing group: II Proper shipping name: Toxic liquid, organic, n.o.s. (Toluene-α-thiol)

15. REGULATORY INFORMATION

SARA 302 Components

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SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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

	CAS-No.	Revision Date
Toluene-α-thiol	100-53-8	1993-04-24

Pennsylvania Right To Know Components

CAS-No. Revision Date Toluene-α-thiol 100-53-8 1993-04-24

New Jersey Right To Know Components

CAS-No.Revision DateToluene-α-thiol100-53-81993-04-24

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

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox. Acute toxicity
Flam. Liq. Flammable liquids
H227 Combustible liquid
H302 Harmful if swallowed.

H330 Fatal if inhaled.

HMIS Rating

Health hazard: 4
Chronic Health Hazard: Flammability: 2
Physical Hazard 0

NFPA Rating

Health hazard: 4
Fire Hazard: 2
Reactivity Hazard: 0

Further information

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Preparation Information

Sigma-Aldrich Corporation Product Safety – Americas Region 1-800-521-8956

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