SAFETY DATA SHEET

Version 3.16
Revision Date 08/31/2018
Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Benzenethiol

Product Number : W361607
Brand : Aldrich

CAS-No. : 108-98-5

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

Identified uses : Laboratory chemicals, Synthesis 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 # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquids (Category 3), H226
Acute toxicity, Oral (Category 2), H300
Acute toxicity, Inhalation (Category 1), H330
Acute toxicity, Dermal (Category 2), H310
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319
Reproductive toxicity (Category 2), H361
Specific target organ toxicity - single exposure, Oral (Category 2), Nervous system, H371
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Specific target organ toxicity - repeated exposure, Oral (Category 1), Kidney, H372
Acute aquatic toxicity (Category 1), H400
Chronic aquatic toxicity (Category 1), H410

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)

H226	Flammable liquid and vapour.
H300 + H310 + H330	Fatal if swallowed, in contact with skin or if inhaled.
H315	Causes skin irritation.
H319	Causes serious eye irritation.

H335	May cause respiratory irritation.
H361	Suspected of damaging fertility or the unborn child.
H371	May cause damage to organs (Nervous system) if swallowed.
H372	Causes damage to organs (Kidney) through prolonged or repeated exposure if swallowed.
H410	Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260	Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P262	Do not get in eyes, on skin, or on clothing.
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.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P284	Wear respiratory protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/doctor. Rinse mouth.
P302 + P350 + P310	IF ON SKIN: Gently wash with plenty of soap and water. Immediately call a POISON CENTER or doctor/ physician.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P311	IF exposed or concerned: Call a POISON CENTER/doctor.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391	Collect spillage.
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	:	Phenyl mercaptan Thiophenol Benzenethiol
Formula	:	C_6H_6S
Molecular weight	:	110.18 g/mol
CAS-No.	:	108-98-5

EC-No. : 203-635-3

Hazardous components

Component	Classification	Concentration
Benzenethiol		
	Flam. Liq. 3; Acute Tox. 2; Acute Tox. 1; Acute Tox. 2; Skin Irrit. 2; Eye Irrit. 2A; Repr. 2; STOT SE 2; STOT SE 3; STOT RE 1; Aquatic Acute 1; Aquatic Chronic 1; H226, H300 + H310 + H330, H315, H319, H335, H361, H371, H372, H410	90 - 100 %

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
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.

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

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
Dry powder Dry sand

Unsuitable extinguishing media
Do NOT use water jet.

5.2 Special hazards arising from the substance or mixture
No data available

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting 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. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

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.
Storage class (TRGS 510): 3: Flammable liquids

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

Component	CAS-No.	Value	Control parameters	Basis
Benzenethiol	108-98-5	TWA	0.1 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Central Nervous System impairment Eye irritation Skin irritation Danger of cutaneous absorption		
		C	0.1 ppm 0.5 mg/m3	USA. NIOSH Recommended Exposure Limits
		15 minute ceiling value		
		PEL	0.5 ppm 2 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

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).

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.

Full contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested:Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Splash contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested:Vitoject® (KCL 890 / Aldrich Z677698, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

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.

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).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: clear, liquid Colour: colourless
b)	Odour	Stench.
c)	Odour Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point/range: -15 °C (5 °F) - lit.
f)	Initial boiling point and boiling range	169 °C (336 °F) - lit.
g)	Flash point	50 °C (122 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapour pressure	4.5 hPa (3.4 mmHg) at 40 °C (104 °F) 1.9 hPa (1.4 mmHg) at 20 °C (68 °F)

l)	Vapour density	3.8 - (Air = 1.0)
m)	Relative density	1.073 g/cm3 at 25 °C (77 °F)
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Auto-ignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information

Relative vapour density 3.8 - (Air = 1.0)

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

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulphur oxides
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - 46.2 mg/kg
Remarks: Behavioral:Somnolence (general depressed activity). Behavioral:Coma. Respiratory disorder

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.

LD50 Dermal - Rabbit - 134 mg/kg
Remarks: Behavioral:Muscle weakness. Behavioral:Ataxia. Cyanosis

No data available

Skin corrosion/irritation
Serious eye damage/eye irritation
No data available

Respiratory or skin sensitisation
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.

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 on OSHA's list of regulated carcinogens.

Reproductive toxicity
Some evidence of adverse effects on sexual function and fertility, and/or on development, based on animal experiments.

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

Specific target organ toxicity - single exposure
Oral - The substance or mixture is classified as specific target organ toxicant, single exposure, category 2. - Nervous system
The substance or mixture is classified as specific target organ toxicant, single exposure, category 3 with respiratory tract irritation.

Specific target organ toxicity - repeated exposure
Oral - The substance or mixture is classified as specific target organ toxicant, repeated exposure, category 1. - Kidney

Aspiration hazard
No data available

Additional Information
RTECS: DC0525000

Cough, Shortness of breath, Headache, Nausea, Vomiting

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	LC50 - Oryzias latipes (Japanese medaka) - 0.009 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 0.0044 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	EC50 - Pseudokirchneriella subcapitata (green algae) - 0.211 mg/l - 72 h (OECD Test Guideline 201)

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
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Very toxic to aquatic life with long lasting effects.

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

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

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
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

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

SARA 302 Components

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

SARA 313 Components
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, Chronic Health Hazard

Massachusetts Right To Know Components

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

Pennsylvania Right To Know Components

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

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
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids

H226	Flammable liquid and vapour.
H300	Fatal if swallowed.
H300 + H310 + H330	Fatal if swallowed, in contact with skin or if inhaled.
H310	Fatal in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H330	Fatal if inhaled.
H335	May cause respiratory irritation.
H361	Suspected of damaging fertility or the unborn child.
H371	May cause damage to organs if swallowed.
H372	Causes damage to organs (/$/*_ORG_REP_ORAL/$/) through prolonged or repeated exposure if swallowed.

Further information

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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

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

Version: 3.16 Revision Date: 08/31/2018 Print Date: 11/10/2018