

## SAFETY DATA SHEET

Creation Date 23-Apr-2010

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Revision Number 4

### 1. Identification

**Product Name** Thiophenol

**Cat No. :** A15916

**CAS No** 108-98-5  
**Synonyms** Phenyl mercaptan; Benzenethiol

**Recommended Use** Laboratory chemicals.  
**Uses advised against** Food, drug, pesticide or biocidal product use.

#### Details of the supplier of the safety data sheet

##### Company

Thermo Fisher Scientific Chemicals, Inc.  
30 Bond Street  
Ward Hill, MA 01835-8099  
Tel: 800-343-0660  
Fax: 800-322-4757

##### **Emergency Telephone Number**

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

### 2. Hazard(s) identification

#### **Classification**

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 3
Acute oral toxicity	Category 2
Acute dermal toxicity	Category 2
Acute Inhalation Toxicity - Vapors	Category 1
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Reproductive Toxicity	Category 2
Specific target organ toxicity (single exposure)	Category 2
Target Organs - Respiratory system, Central nervous system (CNS).	
Specific target organ toxicity - (repeated exposure)	Category 1
Target Organs - Liver, Kidney, spleen.	

#### Label Elements

**Signal Word**

Danger

**Hazard Statements**

Flammable liquid and vapor  
Causes skin irritation  
Causes serious eye irritation  
May cause respiratory irritation  
Suspected of damaging fertility or the unborn child  
May cause damage to organs  
Causes damage to organs through prolonged or repeated exposure  
Fatal if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

Obtain special instructions before use  
Do not handle until all safety precautions have been read and understood  
Use personal protective equipment as required  
Wash face, hands and any exposed skin thoroughly after handling  
Do not eat, drink or smoke when using this product  
Do not get in eyes, on skin, or on clothing  
Do not breathe dust/fume/gas/mist/vapors/spray  
Use only outdoors or in a well-ventilated area  
Wear respiratory protection  
Wear eye/face protection  
Keep away from heat/sparks/open flames/hot surfaces. - No smoking  
Keep container tightly closed  
Ground/bond container and receiving equipment  
Use explosion-proof electrical/ventilating/lighting equipment  
Use only non-sparking tools  
Take precautionary measures against static discharge  
Keep cool

**Response**

IF exposed or concerned: Get medical attention/advice

**Inhalation**

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing  
Immediately call a POISON CENTER or doctor/physician

**Skin**

Immediately call a POISON CENTER or doctor/physician  
Wash contaminated clothing before reuse  
If skin irritation occurs: Get medical advice/attention  
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower

**Eyes**

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

**Ingestion**

IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician  
Rinse mouth

**Fire**

In case of fire: Use CO<sub>2</sub>, dry chemical, or foam for extinction

**Storage**

Store locked up  
Store in a well-ventilated place. Keep container tightly closed

**Disposal**

Dispose of contents/container to an approved waste disposal plant

**Hazards not otherwise classified (HNOC)**

Very toxic to aquatic life with long lasting effects

**Other hazards**

Stench.

### 3. Composition/Information on Ingredients

Component	CAS No	Weight %
Benzenethiol	108-98-5	>95

### 4. First-aid measures

<b>General Advice</b>	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Inhalation</b>	Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately.
<b>Most important symptoms and effects</b>	None reasonably foreseeable. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
<b>Notes to Physician</b>	Treat symptomatically

### 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Water spray, carbon dioxide (CO <sub>2</sub> ), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.
<b>Unsuitable Extinguishing Media</b>	Do not use a solid water stream as it may scatter and spread fire
<b>Flash Point</b>	50 °C / 122 °F
<b>Method -</b>	No information available
<b>Autoignition Temperature</b>	450 °C / 842 °F
<b>Explosion Limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Sensitivity to Mechanical Impact</b>	No information available
<b>Sensitivity to Static Discharge</b>	No information available

**Specific Hazards Arising from the Chemical**

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of

ignition and flash back. Do not allow run-off from fire-fighting to enter drains or water courses.

### Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Sulfur oxides.

### Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

### NFPA

Health  
4

Flammability  
2

Instability  
1

Physical hazards  
N/A

## 6. Accidental release measures

### Personal Precautions

Use personal protective equipment as required. Ensure adequate ventilation. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas. Remove all sources of ignition. Take precautionary measures against static discharges.

### Environmental Precautions

Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

### Methods for Containment and Clean Up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

## 7. Handling and storage

### Handling

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.

### Storage.

Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame. Store under an inert atmosphere. Incompatible Materials. Strong oxidizing agents. Acids.

## 8. Exposure controls / personal protection

### Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
Benzenethiol	TWA: 0.1 ppm Skin	(Vacated) TWA: 0.5 ppm (Vacated) TWA: 2 mg/m <sup>3</sup>	Ceiling: 0.1 ppm Ceiling: 0.5 mg/m <sup>3</sup>	TWA: 0.1 ppm

### Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

### Engineering Measures

Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting equipment. Ensure adequate ventilation, especially in confined areas.

### Personal Protective Equipment

#### Eye/face Protection

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166. Tight sealing safety goggles. Face protection shield.

#### Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

**Respiratory Protection** Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

**Recommended Filter type:** Organic gases and vapours filter. Type A. Brown. conforming to EN14387.

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

## 9. Physical and chemical properties

Physical State	Liquid
Appearance	Clear
Odor	Stench
Odor Threshold	No information available
pH	5 saturated solution
Melting Point/Range	-15 °C / 5 °F
Boiling Point/Range	167 - 169 °C / 332.6 - 336.2 °F @ 760 mmHg
Flash Point	50 °C / 122 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	1.6 mmHg @ 25 °C
Vapor Density	No information available
Specific Gravity	1.078
Solubility	Insoluble in water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	450 °C / 842 °F
Decomposition Temperature	> 200°C
Viscosity	0.981cSt at 30 °C
Molecular Formula	C6 H6 S
Molecular Weight	110.17

## 10. Stability and reactivity

<b>Reactive Hazard</b>	None known, based on information available
<b>Stability</b>	Air sensitive.
<b>Conditions to Avoid</b>	Incompatible products. Excess heat. Exposure to air. Keep away from open flames, hot surfaces and sources of ignition.
<b>Incompatible Materials</b>	Strong oxidizing agents, Acids
<b>Hazardous Decomposition Products</b>	Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> ), Sulfur oxides
<b>Hazardous Polymerization</b>	Hazardous polymerization does not occur.
<b>Hazardous Reactions</b>	None under normal processing.

## 11. Toxicological information

### Acute Toxicity

<b>Product Information</b>	
Oral LD50	Category 2.
Dermal LD50	Category 2.
Vapor LC50	Category 1.
<b>Component Information</b>	

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzenethiol	46 mg/kg ( Rat )	134 mg/kg ( Rabbit ) 300 mg/kg ( Rat )	LC50 = 33 ppm ( Rat ) 4 h

**Toxicologically Synergistic Products** No information available

**Delayed and immediate effects as well as chronic effects from short and long-term exposure**

**Irritation** Irritating to eyes, respiratory system and skin

**Sensitization** No information available

**Carcinogenicity** The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Benzenethiol	108-98-5	Not listed	Not listed	Not listed	Not listed	Not listed

**Mutagenic Effects** No information available

**Reproductive Effects** No information available.

**Developmental Effects** No information available.

**Teratogenicity** No information available.

**STOT - single exposure** Respiratory system Central nervous system (CNS)

**STOT - repeated exposure** Liver Kidney spleen

**Aspiration hazard** No information available

**Symptoms / effects, both acute and delayed** Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

**Endocrine Disruptor Information** No information available

**Other Adverse Effects** The toxicological properties have not been fully investigated.

## 12. Ecological information

### Ecotoxicity

Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Benzenethiol	Not listed	Not listed	EC50 = 0.875 mg/L 15 min EC50 = 0.875 mg/L 30 min EC50 = 0.875 mg/L 5 min	EC50 = 0.0044 mg/L 48h

**Persistence and Degradability** Persistence is unlikely

**Bioaccumulation/ Accumulation** No information available.

**Mobility** . Is not likely mobile in the environment due its low water solubility.

Component	log Pow
Benzenethiol	2.52

## 13. Disposal considerations

**Waste Disposal Methods** Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

## 14. Transport information

**DOT**

UN-No UN2337  
 Proper Shipping Name PHENYL MERCAPTAN  
 Hazard Class 6.1  
 Subsidiary Hazard Class 3  
 Packing Group I

**TDG**

UN-No UN2337  
 Proper Shipping Name PHENYL MERCAPTAN  
 Hazard Class 6.1  
 Subsidiary Hazard Class 3  
 Packing Group I

**IATA**

UN-No UN2337  
 Proper Shipping Name Phenyl mercaptan, FORBIDDEN FOR IATA TRANSPORT  
 Hazard Class 6.1  
 Subsidiary Hazard Class 3  
 Packing Group I

**IMDG/IMO**

UN-No UN2337  
 Proper Shipping Name Phenyl mercaptan  
 Hazard Class 6.1  
 Subsidiary Hazard Class 3  
 Packing Group I

## 15. Regulatory information

**United States of America Inventory**

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Benzenethiol	108-98-5	X	ACTIVE	-

**Legend:**

**TSCA** US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

**TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)**

Not applicable

**TSCA 12(b)** - Notices of Export

Not applicable

**International Inventories**

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Benzenethiol	108-98-5	X	-	203-635-3	X	X	X	X	X	KE-33799

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

**U.S. Federal Regulations****SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

**SARA 311/312 Hazard Categories**

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate

classifications.

**CWA (Clean Water Act)** Not applicable

**Clean Air Act** Not applicable

**OSHA - Occupational Safety and Health Administration** Not applicable

**CERCLA**

This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355).

Component	Hazardous Substances RQs	CERCLA Extremely Hazardous Substances RQs	SARA Reportable Quantity (RQ)
Benzenethiol	100 lb	100 lb	100 lb 45.4 kg

**California Proposition 65** This product does not contain any Proposition 65 chemicals.

**U.S. State Right-to-Know Regulations**

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Benzenethiol	X	X	X	X	X

**U.S. Department of Transportation**

Reportable Quantity (RQ): Y

DOT Marine Pollutant N

DOT Severe Marine Pollutant N

**U.S. Department of Homeland Security** This product does not contain any DHS chemicals.

**Other International Regulations**

**Mexico - Grade** Moderate risk, Grade 2

**Authorisation/Restrictions according to EU REACH** Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Benzenethiol	108-98-5	-	-	-

**Safety, health and environmental regulations/legislation specific for the substance or mixture**

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Benzenethiol	108-98-5	Not applicable	Not applicable	Not applicable	Not applicable

**Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?**

Not applicable



## Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Benzenethiol	108-98-5	Not applicable	Not applicable	Not applicable	Not applicable

## 16. Other information

**Prepared By** Health, Safety and Environmental Department  
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www.thermofisher.com

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**Revision Summary** New emergency telephone response service provider.

## Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of SDS**