

SAFETY DATA SHEET

Creation Date 30-Apr-2012

Revision Date 26-Dec-2021

Revision Number 5

1. Identification

Product Name Benzyl mercaptan

Cat No. : AC421260000; AC421260050; AC421260250; AC421261000;
AC421265000

CAS No 100-53-8
Synonyms alpha-Toluenetiol; Thiobenzyl alcohol

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

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number For information **US** call: 001-800-ACROS-01 / **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 4
Acute oral toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 2
Serious Eye Damage/Eye Irritation	Category 2

Label Elements

Signal Word
Danger

Hazard Statements
Combustible liquid
Harmful if swallowed

Causes serious eye irritation
Fatal if inhaled



Precautionary Statements

Prevention

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Do not breathe dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Wear respiratory protection
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Wear protective gloves/protective clothing/eye protection/face protection
Keep cool

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

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: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth

Fire

In case of fire: Use CO₂, dry chemical, or foam for extinction

Storage

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

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 %
Benzyl mercaptan	100-53-8	>95

4. First-aid measures

General Advice

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

Eye Contact

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.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical

	attention is required.
Inhalation	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.
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.
Most important symptoms and effects	None reasonably foreseeable. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	Do not use a solid water stream as it may scatter and spread fire
Flash Point	70 °C / 158 °F
Method -	No information available
Autoignition Temperature	270 °C / 518 °F
Explosion Limits	
Upper	No data available
Lower	1%
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Combustible material. Keep product and empty container away from heat and sources of ignition. Risk of ignition. Containers may explode when heated. Do not allow run-off from fire-fighting to enter drains or water courses.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Sulfur oxides. Sulfides.

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	Flammability	Instability	Physical hazards
4	2	1	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	Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition.

7. Handling and storage

Handling	Do not get in eyes, on skin, or on clothing. Wear personal protective equipment/face protection. 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.
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. Acids. Strong oxidizing agents. Strong bases.

8. Exposure controls / personal protection

Exposure Guidelines	This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.
Engineering Measures	Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.
Personal Protective Equipment	
Eye/face Protection	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.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Light yellow
Odor	Stench
Odor Threshold	No information available
pH	No information available
Melting Point/Range	-29 °C / -20.2 °F
Boiling Point/Range	195 °C / 383 °F
Flash Point	70 °C / 158 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	1%
Vapor Pressure	0.5 mbar @ 20 °C
Vapor Density	4.28
Specific Gravity	1.058
Solubility	Insoluble in water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	270 °C / 518 °F
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C7 H8 S
Molecular Weight	124.21

10. Stability and reactivity

Reactive Hazard	None known, based on information available
------------------------	--------------------------------------------

Stability	Air sensitive.
Conditions to Avoid	Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition. Exposure to air.
Incompatible Materials	Acids, Strong oxidizing agents, Strong bases
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂), Sulfur oxides, Sulfides
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzyl mercaptan	493 mg/kg (Rat)	> 2000 mg/kg (Rabbit)	178 ppm (4h) (Mouse)

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

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
Benzyl mercaptan	100-53-8	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects Not mutagenic in AMES Test

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure None known
STOT - repeated exposure None known

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
-----------	------------------	-----------------	----------	------------

Benzyl mercaptan	Not listed	Not listed	EC50 = 0.96 mg/L 5 min EC50 = 0.99 mg/L 15 min EC50 = 1.21 mg/L 30 min	Not listed
------------------	------------	------------	------------------------------------------------------------------------------	------------

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
Benzyl mercaptan	2.48

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 UN2810
 Proper Shipping Name Toxic liquid, organic, n.o.s.
 Technical Name (ALPHA-TOLUENETHIOL)
 Hazard Class 6.1
 Packing Group II

TDG

UN-No UN2810
 Proper Shipping Name Toxic liquid, organic, n.o.s.
 Hazard Class 6.1
 Packing Group II

IATA

UN-No UN2810
 Proper Shipping Name Toxic liquid, organic, n.o.s.
 Hazard Class 6.1
 Packing Group II

IMDG/IMO

UN-No UN2810
 Proper Shipping Name Toxic liquid, organic, n.o.s.
 Hazard Class 6.1
 Packing Group II

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Benzyl mercaptan	100-53-8	X	ACTIVE	SP;TP

Legend:

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

X - Listed

'-' - Not Listed

SP - Indicates a substance that is identified in a proposed SNUR

TSCA 12(b) - Notices of Export

Component	CAS No	TSCA 12(b) - Notices of Export
Benzyl mercaptan	100-53-8	Section 5

International Inventories

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

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Benzyl mercaptan	100-53-8	X	-	202-862-5	X	X	X	X	X	-

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

U.S. Federal Regulations

SARA 313	Not applicable
SARA 311/312 Hazard Categories	See section 2 for more information
CWA (Clean Water Act)	Not applicable
Clean Air Act	Not applicable
OSHA - Occupational Safety and Health Administration	Not applicable
CERCLA	Not applicable

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
Benzyl mercaptan	X	-	X	-	-

U.S. Department of Transportation

Reportable Quantity (RQ):	N
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

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)
Benzyl mercaptan	100-53-8	Listed	Not applicable	Not applicable	Not applicable

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)
Benzyl mercaptan	100-53-8	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By	Regulatory Affairs Thermo Fisher Scientific Email: EMSDS.RA@thermofisher.com
Creation Date	30-Apr-2012
Revision Date	26-Dec-2021
Print Date	26-Dec-2021
Revision Summary	This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

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