

SAFETY DATA SHEET

Creation Date 22-Sep-2009

Revision Date 18-Dec-2025

Revision Number 8

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

Product Name Thioanisole

Cat No. : AC138670000; AC138670025; AC138670250; AC138671000; AC138675000

CAS No 100-68-5
Synonyms MPS; Methyl phenyl sulfide

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: 001-800-227-6701 / **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 according to [US] OSHA (29 CFR 1910.1200, 2024)

Flammable liquids	Category 4
Acute oral toxicity	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Skin Sensitization	Category 1

Label Elements

Signal Word

Warning

Hazard Statements

Combustible liquid
Harmful if swallowed
Causes skin irritation
Causes serious eye irritation
May cause an allergic skin reaction

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Wear protective gloves/protective clothing/eye protection/face protection
Avoid breathing dust/fume/gas/mist/vapors/spray
Contaminated work clothing should not be allowed out of the workplace
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

Skin

IF ON SKIN: Wash with plenty of soap and water
Take off contaminated clothing
If skin irritation or rash occurs: Get medical advice/attention

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 to extinguish

Storage

Store in a well-ventilated place. Keep cool

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

Toxic to aquatic life with long lasting effects

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

Other hazards

Stench.

3. Composition/information on Ingredients

Component	CAS No	Weight %
Benzene, (methylthio)-	100-68-5	>95

4. First-aid measures

General Advice

If symptoms persist, call a physician.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Most important symptoms and effects	None reasonably foreseeable. May cause allergic skin reaction. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing
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	No information available
Flash Point	73 °C / 163.4 °F
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Flammable. Keep product and empty container away from heat and sources of ignition. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Combustible material.

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.

NFPA

Health
2

Flammability
2

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions	Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.
Environmental Precautions	Do not flush into surface water or sanitary sewer system.
Methods for Containment and Clean Up	Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition.

7. Handling and Storage

Handling	Ensure adequate ventilation. Wear personal protective equipment/face protection. Avoid ingestion and inhalation. Do not get in eyes, on skin, or on clothing. Keep away from open
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flames, hot surfaces and sources of ignition.

Storage.

Keep away from heat, sparks and flame. Flammables area. Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Strong oxidizing agents.

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. Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location.

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.

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection

No protective equipment is needed under normal use conditions.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance**Physical State**

Liquid

Color

Light yellow

Odor

Stench

Odor Threshold

No information available

Property**Values****Remarks****• Method****Melting Point/Range**

-15 °C / 5 °F

Softening Point

No data available

Boiling Point/Range

188 °C / 370.4 °F

Flash Point

73 °C / 163.4 °F

Flammability (liquid)

Combustible liquid

Flammability (solid,gas)

Not applicable

Explosion Limits

No data available

@ 760 mmHg

Method - No information available

On basis of test data

Liquid

Autoignition Temperature

No data available

Decomposition Temperature

No data available

pH

No information available

Viscosity

No data available

Water Solubility

Insoluble

Solubility in other solvents

No information available

Partition Coefficient (n-octanol/water)**Component****log Pow**

Benzene, (methylthio)-

2.9

Vapor Pressure

No data available

Density / Specific Gravity

1.050

Bulk Density

Not applicable

Liquid

Vapor Density

4.3

(Air = 1.0)

Particle characteristics

Not applicable (liquid)

Other Information**Molecular Formula**

C7 H8 S

Molecular Weight

124.2

Explosive Properties

explosive air/vapour mixtures possible

10. Stability and reactivity**Reactive Hazard**

None known, based on information available

Stability

Stable under normal conditions.

Conditions to Avoid

Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.

Incompatible Materials

Strong oxidizing agents

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO₂), Sulfur oxides, Sulfides**Hazardous Polymerization**

Hazardous polymerization does not occur.

Hazardous Reactions

None under normal processing.

11. Toxicological information**Information on expected route of exposure****Inhalation**

May produce an allergic reaction.

Ingestion

May cause allergic reaction. May be harmful if swallowed.

Eyes

Avoid contact with eyes. Irritating to eyes. Sensitization.

Skin

Avoid contact with skin. May cause irritation. Repeated or prolonged skin contact may cause allergic reactions with susceptible persons.

Toxicology data for the components

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzene, (methylthio)-	LD50 = 891 mg/kg (Rat)	-	-

Toxicologically Synergistic Products

No information available

(b) skin corrosion/irritation;

Category 2

(c) serious eye damage/irritation;

Category 2

(d) respiratory or skin sensitization;**Respiratory**

No data available

Skin

Category 1

May cause sensitization by skin contact

(e) germ cell mutagenicity;

No data available

(f) carcinogenicity;

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

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Benzene, (methylthio)-	100-68-5	Not listed	Not listed	Not listed	Not listed	Not listed

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs None known.

(j) aspiration hazard; No data available

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing.

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

Endocrine Disrupting Properties This product does not contain any known or suspected endocrine disruptors.

12. Ecological information

Ecotoxicity

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
Benzene, (methylthio)-	Not listed	Not listed	Not listed	EC50: 2.2-4.0 mg/L/24h

Persistence and Degradability Insoluble in water May persist based on information available.

Bioaccumulation/ Accumulation No information available.

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

Component	log Pow
Benzene, (methylthio)-	2.9

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 UN3082
 Proper Shipping Name Environmentally hazardous substances, liquid, n.o.s.
 Technical Shipping Name Benzene, (methylthio)-
 Hazard Class 9
 Packing Group III

TDG

UN-No UN3082
 Proper Shipping Name Environmentally hazardous substances, liquid, n.o.s.
 Technical Shipping Name Benzene, (methylthio)-
 Hazard Class 9
 Packing Group III

IATA

UN-No UN3082
 Proper Shipping Name Environmentally hazardous substances, liquid, n.o.s.
 Technical Shipping Name Benzene, (methylthio)-
 Hazard Class 9
 Packing Group III

IMDG/IMO

UN-No UN3082
 Proper Shipping Name Environmentally hazardous substances, liquid, n.o.s.
 Technical Shipping Name Benzene, (methylthio)-
 Hazard Class 9
 Packing Group III

15. Regulatory Information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Benzene, (methylthio)-	100-68-5	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

China, X = listed, Australia, U.S.A. (TSCA), Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Australia (AICS), Korea (KECL), China (IECSC), Japan (ENCS), Philippines (PICCS).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Benzene, (methylthio)-	100-68-5	-	X	202-878-2	X	X	X	X	X	2000-3-1441

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, does not contain any substances regulated as hazardous substances under the Comprehensive

Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

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

U.S. State Right-to-Know Regulations Not applicable

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 No information available

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)
Benzene, (methylthio)-	100-68-5	-	-	-

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)
Benzene, (methylthio)-	100-68-5	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)
Benzene, (methylthio)-	100-68-5	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information

Prepared By

Product stewardship (Regulatory Affairs)
Thermo Fisher Scientific
email - begel.sdsdesk@thermofisher.com

Creation Date	22-Sep-2009
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Print Date	18-Dec-2025
Revision Summary	Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

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