

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

| | |
|-----------------------------|---|
| Product Description: | Thioanisole |
| Cat No. : | 138670000; 138670250; 138671000; 138675000 |
| Synonyms | MPS; Methyl phenyl sulfide |
| CAS No | 100-68-5 |
| EC No | 202-878-2 |
| Molecular Formula | C7 H8 S |

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

| | |
|-----------------------------|--------------------------|
| Recommended Use | Laboratory chemicals. |
| Uses advised against | No Information available |

1.3. Details of the supplier of the safety data sheet

Company

UK entity/business name
Fisher Scientific UK
Bishop Meadow Road,
Loughborough, Leicestershire LE11 5RG, United Kingdom

EU entity/business name
Thermo Fisher Scientific
Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium

E-mail address begel.sdsdesk@thermofisher.com

1.4. 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

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

Physical hazards

Based on available data, the classification criteria are not met

Health hazards

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| | |
|-----------------------------------|-------------------|
| Acute oral toxicity | Category 4 (H302) |
| Skin Corrosion/Irritation | Category 2 (H315) |
| Serious Eye Damage/Eye Irritation | Category 2 (H319) |
| Skin Sensitization | Category 1 (H317) |
| Environmental hazards | |
| Chronic aquatic toxicity | Category 2 (H411) |

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Warning

Hazard Statements

H302 - Harmful if swallowed
H319 - Causes serious eye irritation
H411 - Toxic to aquatic life with long lasting effects
H315 - Causes skin irritation
H317 - May cause an allergic skin reaction
Combustible liquid

Precautionary Statements

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting
P312 - Call a POISON CENTER or doctor if you feel unwell
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P280 - Wear protective gloves/protective clothing/eye protection/face protection

2.3. Other hazards

Stench
Toxic to terrestrial vertebrates
This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

| Component | CAS No | EC No | Weight % | CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567 |
|------------------------|----------|-------------------|----------|---|
| Benzene, (methylthio)- | 100-68-5 | EEC No. 202-878-2 | >95 | Acute Tox. 4 (H302) Skin Irrit. 2 (H315) |

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| | | | | |
|--|--|--|--|--|
| | | | | Eye Irrit. 2 (H319) Skin Sens. 1 (H317) Aquatic Chronic 2 (H411) |
|--|--|--|--|--|

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of 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. |
| Ingestion | Clean mouth with water and drink afterwards plenty of water. |
| Inhalation | Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. |
| Self-Protection of the First Aider | No special precautions required. |

4.2. Most important symptoms and effects, both acute and delayed

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

4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician Treat symptomatically.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

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.

5.3. Advice for firefighters

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As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

6.2. Environmental precautions

Do not flush into surface water or sanitary sewer system.

6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe 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 flames, hot surfaces and sources of ignition.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

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

Technical Rules for Hazardous Substances (TRGS) 510 Class 10
Storage Class (LGK) (Germany)

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

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Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

Predicted No Effect Concentration (PNEC)

See values below.

| Component | Fresh water | Fresh water sediment | Water Intermittent | Microorganisms in sewage treatment | Soil (Agriculture) |
|--------------------------------------|-------------------|----------------------|--------------------|------------------------------------|--------------------|
| Benzene, (methylthio)-100-68-5 (>95) | PNEC = 0.0013mg/L | | PNEC = 0.013mg/L | | |

| Component | Marine water | Marine water sediment | Marine water intermittent | Food chain | Air |
|--------------------------------------|--------------------|-----------------------|---------------------------|------------|-----|
| Benzene, (methylthio)-100-68-5 (>95) | PNEC = 0.00013mg/L | | | | |

8.2. Exposure controls

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.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

| Glove material | Breakthrough time | Glove thickness | EU standard | Glove comments |
|----------------|-----------------------------------|-----------------|-------------|-----------------------|
| Nitrile rubber | See manufacturers recommendations | - | EN 374 | (minimum requirement) |
| Neoprene | | | | |
| Natural rubber | | | | |
| PVC | | | | |

Skin and body protection Long sleeved clothing.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Respiratory Protection No protective equipment is needed under normal use conditions.

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

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Small scale/Laboratory use Maintain adequate ventilation

Environmental exposure controls Prevent product from entering drains. Do not allow material to contaminate ground water system.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

| | | |
|--|--------------------------|--|
| Physical State | Liquid | |
| Appearance | Light yellow | |
| Odor | Stench | |
| Odor Threshold | No data available | |
| Melting Point/Range | -15 °C / 5 °F | |
| Softening Point | No data available | |
| Boiling Point/Range | 188 °C / 370.4 °F | @ 760 mmHg |
| Flammability (liquid) | Combustible liquid | On basis of test data |
| Flammability (solid,gas) | Not applicable | Liquid |
| Explosion Limits | No data available | |
| Flash Point | 73 °C / 163.4 °F | Method - No information available |
| 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 (Air = 1.0) |
| Vapor Density | 4.3 | |
| Particle characteristics | Not applicable (liquid) | |

9.2. Other information

| | |
|-----------------------------|--|
| Molecular Formula | C7 H8 S |
| Molecular Weight | 124.2 |
| Explosive Properties | explosive air/vapour mixtures possible |

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity None known, based on information available

10.2. Chemical stability Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous Polymerization No information available.
Hazardous Reactions None under normal processing.

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10.4. Conditions to avoid

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

10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

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

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

(a) acute toxicity;

| | |
|------------|-------------------|
| Oral | Category 4 |
| Dermal | No data available |
| Inhalation | No data available |

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

(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; No data available
There are no known carcinogenic chemicals in this product

(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

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of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing.

11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects

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 Fish | Water Flea | Freshwater Algae |
|------------------------|-----------------|------------------------|------------------|
| Benzene, (methylthio)- | | EC50: 2.2-4.0 mg/L/24h | |

12.2. Persistence and degradability

Persistence

Not readily biodegradable
Insoluble in water, May persist, based on information available.

Degradation in sewage treatment plant

Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

12.3. Bioaccumulative potential

May have some potential to bioaccumulate

| Component | log Pow | Bioconcentration factor (BCF) |
|------------------------|---------|-------------------------------|
| Benzene, (methylthio)- | 2.9 | No data available |

12.4. Mobility in soil

Spillage unlikely to penetrate soil The product is insoluble and sinks in water The product evaporates slowly Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil

12.5. Results of PBT and vPvB assessment

No data available for assessment.

12.6. Endocrine disrupting properties

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

Persistent Organic Pollutant Ozone Depletion Potential

This product does not contain any known or suspected substance

This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and

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empty container away from heat and sources of ignition.

European Waste Catalogue (EWC) According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

Other Information Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Do not let this chemical enter the environment.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN3082
14.2. UN proper shipping name Environmentally hazardous substances, liquid, n.o.s.
Technical Shipping Name Benzene, (methylthio)-
14.3. Transport hazard class(es) 9
14.4. Packing group III

ADR

14.1. UN number UN3082
14.2. UN proper shipping name Environmentally hazardous substances, liquid, n.o.s.
Technical Shipping Name Benzene, (methylthio)-
14.3. Transport hazard class(es) 9
14.4. Packing group III

IATA

14.1. UN number UN3082
14.2. UN proper shipping name Environmentally hazardous substances, liquid, n.o.s.
Technical Shipping Name Benzene, (methylthio)-
14.3. Transport hazard class(es) 9
14.4. Packing group III

14.5. Environmental hazards Dangerous for the environment
Product is a marine pollutant according to the criteria set by IMDG/IMO

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

International Inventories

China, X = listed, Australia, U.S.A. (TSCA), Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Australia (AICS), Korea (KECL), China (IECSC), Japan (ENCS), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

| Component | CAS No | EINECS | ELINCS | NLP | IECSC | TCSI | KECL | ENCS | ISHL |
|------------------------|----------|-----------|--------|-----|-------|------|-----------------|------|------|
| Benzene, (methylthio)- | 100-68-5 | 202-878-2 | - | - | X | X | 2000-3-14 41 | X | X |

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| Component | CAS No | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|------------------------|----------|------|---|-----|------|------|-------|-------|
| Benzene, (methylthio)- | 100-68-5 | X | ACTIVE | - | X | X | X | X |

Legend: X - Listed '-' - Not Listed

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

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 | - | - | - |

Seveso III Directive (2012/18/EC)

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

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

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

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification

Water endangering class = 2 (self classification)

| Component | Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81) | Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC) | Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure |
|--|--|---|---|
| Benzene, (methylthio)- 100-68-5 (>95) | Prohibited and Restricted Substances | | |

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

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SECTION 16: OTHER INFORMATION

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

H302 - Harmful if swallowed
H319 - Causes serious eye irritation
H411 - Toxic to aquatic life with long lasting effects
H315 - Causes skin irritation
H317 - May cause an allergic skin reaction

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Creation Date 22-Sep-2009
Revision Date 25-Sep-2023
Revision Summary Not applicable.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

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

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End of Safety Data Sheet