

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

### 1.1. Product identifier

**Product Description:** 2-Methyl-5-tert-butylthiophenol, remainder isomer  
**Cat No. :** 279960000; 279960500  
**Synonyms** 5-(1,1-Dimethylethyl)-2-methylthiophenol; 2-Methyl-5-(1,1-dimethylethyl)thiophenol  
**Index No** 604-089-00-2  
**CAS No** 7340-90-1  
**EC No** 438-520-9,444-970-7  
**Molecular Formula** C11 H16 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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Aspiration Toxicity	Category 1 (H304)
Skin Corrosion/Irritation	Category 2 (H315)
Serious Eye Damage/Eye Irritation	Category 2 (H319)
Skin Sensitization	Category 1 (H317)
Reproductive Toxicity	Category 2 (H361d)
Specific target organ toxicity - (single exposure)	Category 3 (H336)
Specific target organ toxicity - (repeated exposure)	Category 2 (H373)
<b>Environmental hazards</b>	
Chronic aquatic toxicity	Category 1 (H410)

Full text of Hazard Statements: see section 16

## 2.2. Label elements



Signal Word

Danger

## Hazard Statements

- H319 - Causes serious eye irritation
- H315 - Causes skin irritation
- H361d - Suspected of damaging the unborn child
- H373 - May cause damage to organs through prolonged or repeated exposure
- H304 - May be fatal if swallowed and enters airways
- H317 - May cause an allergic skin reaction
- H336 - May cause drowsiness or dizziness
- H410 - Very toxic to aquatic life with long lasting effects

## Precautionary Statements

- P280 - Wear protective gloves/protective clothing/eye protection/face protection
- P273 - Avoid release to the environment
- P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
- P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

## 2.3. Other hazards

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
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Methyl-2 Tert-Butyle-5 Thiophenol Thio PTBT	7340-90-1	438-520-9,444-970-7	<=100	Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Repr. 2 (H361d) STOT RE 2 (H373) Asp. Tox. 1 (H304) Skin Sens. 1 (H317) STOT SE 3 (H336) Aquatic Chronic 1 (H410) Aquatic Acute 1 (H400)
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Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

<b>General Advice</b>	If symptoms persist, call a physician.
<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
<b>Ingestion</b>	Clean mouth with water and drink afterwards plenty of water. Do NOT induce vomiting. Call a physician or poison control center immediately. If vomiting occurs naturally, have victim lean forward.
<b>Inhalation</b>	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. Risk of serious damage to the lungs (by aspiration).
<b>Self-Protection of the First Aider</b>	Use personal protective equipment as required.

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

May cause allergic skin reaction. 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**

Dry chemical. Foam. Carbon dioxide (CO<sub>2</sub>).

#### **Extinguishing media which must not be used for safety reasons**

No information available.

### 5.2. Special hazards arising from the substance or mixture

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

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## Hazardous Combustion Products

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

### 5.3. Advice for firefighters

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

Use personal protective equipment as required. Ensure adequate ventilation.

### 6.2. 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.

### 6.3. Methods and material for containment and cleaning up

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material.

### 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

Do not get in eyes, on skin, or on clothing. Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid ingestion and inhalation.

#### Hygiene Measures

When using do not eat, drink or smoke. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Provide regular cleaning of equipment, work area and clothing.

### 7.2. Conditions for safe storage, including any incompatibilities

Keep containers tightly closed in a dry, cool and well-ventilated place. Store under an inert atmosphere.

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

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## Exposure limits

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

## 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)

No information available.

## 8.2. Exposure controls

### Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ventilation systems. 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

**Small scale/Laboratory use** Maintain adequate ventilation

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**Environmental exposure controls** 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.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

<b>Physical State</b>	Liquid	
<b>Appearance</b>	Colorless	
<b>Odor</b>	aromatic	
<b>Odor Threshold</b>	No data available	
<b>Melting Point/Range</b>	-10 °C / 14 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	260 °C / 500 °F	@ 760 mmHg
<b>Flammability (liquid)</b>	No data available	
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Flash Point</b>	123 °C / 253.4 °F	<b>Method -</b> No information available
<b>Autoignition Temperature</b>	328 °C / 622.4 °F	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	No information available	
<b>Viscosity</b>	No data available	
<b>Water Solubility</b>	0.0035 g/L (20°C)	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>	No information available	
<b>Vapor Pressure</b>	No information available	
<b>Density / Specific Gravity</b>	0.980	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Vapor Density</b>	No data available	(Air = 1.0)
<b>Particle characteristics</b>	Not applicable (liquid)	

### 9.2. Other information

<b>Molecular Formula</b>	C11 H16 S
<b>Molecular Weight</b>	180.31

## SECTION 10: STABILITY AND REACTIVITY

**10.1. Reactivity** None known, based on information available

**10.2. Chemical stability** Air sensitive.

### 10.3. Possibility of hazardous reactions

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

**10.4. Conditions to avoid** Incompatible products. Exposure to air. Excess heat.

**10.5. Incompatible materials** Strong oxidizing agents.

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## 10.6. Hazardous decomposition products

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

## SECTION 11: TOXICOLOGICAL INFORMATION

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

#### Product Information

##### (a) acute toxicity;

Oral

Based on available data, the classification criteria are not met

Dermal

Based on available data, the classification criteria are not met

Inhalation

Based on available data, the classification criteria are not met

#### Toxicology data for the components

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Methyl-2 Tert-Butyle-5 Thiophenol Thio PTBT	2243 mg/kg (Rat)	>2000 mg/kg (Rabbit)	-

(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;

Reproductive Effects

Category 2

Possible risk of harm to the unborn child.

(h) STOT-single exposure; Category 3

Results / Target organs

Central nervous system (CNS).

(i) STOT-repeated exposure; Category 2

Route of exposure

Oral

Target Organs

Stomach, Liver.

(j) aspiration hazard; Category 1

**Symptoms / effects, both acute and delayed**

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.

### 11.2. Information on other hazards

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**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

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

Component	Freshwater Fish	Water Flea	Freshwater Algae
Methyl-2 Tert-Butyle-5 Thiophenol Thio PTBT	LC50: 3 mg/L/96h (Brachydanio rerio)		

### 12.2. Persistence and degradability

#### Degradation in sewage treatment plant

Not readily biodegradable

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

### 12.3. Bioaccumulative potential

No information available

### 12.4. Mobility in soil

No information available

### 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

Should not be released into the environment. 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.

#### 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.



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## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

<b>14.1. UN number</b>	UN3082
<b>14.2. UN proper shipping name</b> Technical Shipping Name	Environmentally hazardous substances, liquid, n.o.s. 2-Methyl-5-tert-butylthiophenol
<b>14.3. Transport hazard class(es)</b>	9
<b>14.4. Packing group</b>	III

### ADR

<b>14.1. UN number</b>	UN3082
<b>14.2. UN proper shipping name</b> Technical Shipping Name	Environmentally hazardous substances, liquid, n.o.s. 2-Methyl-5-tert-butylthiophenol
<b>14.3. Transport hazard class(es)</b>	9
<b>14.4. Packing group</b>	III

### IATA

<b>14.1. UN number</b>	UN3082
<b>14.2. UN proper shipping name</b> Technical Shipping Name	Environmentally hazardous substances, liquid, n.o.s. 2-Methyl-5-tert-butylthiophenol
<b>14.3. Transport hazard class(es)</b>	9
<b>14.4. Packing group</b>	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

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Methyl-2 Tert-Butyle-5 Thiophenol Thio PTBT	7340-90-1	-	438-520-9, 444-970-7	-	-	X	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Methyl-2 Tert-Butyle-5 Thiophenol Thio PTBT	7340-90-1	-	-	-	-	-	-	-

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

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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)
Methyl-2 Tert-Butyle-5 Thiophenol Thio PTBT	7340-90-1	-	Use restricted. See item 75. (see link for restriction details)	-

**REACH links**

<https://echa.europa.eu/substances-restricted-under-reach>

**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
Methyl-2 Tert-Butyle-5 Thiophenol Thio PTBT	7340-90-1	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 .

Take note of Directive 94/33/EC on the protection of young people at work

Take note of Dir 92/85/EC on the protection of pregnant and breastfeeding women 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 = 3 (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
Methyl-2 Tert-Butyle-5 Thiophenol Thio PTBT 7340-90-1 ( <=100 )	Prohibited and Restricted Substances		

**15.2. Chemical safety assessment**

Chemical Safety Assessment/Reports (CSA/CSR) are not required for mixtures

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## SECTION 16: OTHER INFORMATION

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

H304 - May be fatal if swallowed and enters airways  
H315 - Causes skin irritation  
H317 - May cause an allergic skin reaction  
H319 - Causes serious eye irritation  
H336 - May cause drowsiness or dizziness  
H361d - Suspected of damaging the unborn child  
H400 - Very toxic to aquatic life  
H410 - Very toxic to aquatic life with long lasting effects

### 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

### Classification and procedure used to derive the classification for mixtures according to Regulation (EC) 1272/2008 [CLP]:

**Physical hazards** On basis of test data

**Health Hazards** Calculation method

**Environmental hazards** Calculation method

### 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.

Chemical incident response training.

**Creation Date** 08-Jan-2013

**Revision Date** 29-Sep-2023

**Revision Summary** Not applicable.

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

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## 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 Safety Data Sheet**