

MAYSPB00450

## 3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione

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

产品说明: Product Description:	3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione 3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione
Cat No. : Molecular Formula	SPB00450DA; SPB00450EA; SPB00450SC; SPB00450ZZ C16 H23 N3 O S
Supplier	<b>UK entity/business name</b> Thermo Fisher Scientific (Heysham), Shore Road, Port of Heysham Industrial Park, Heysham, Lancashire, LA3 2XY United Kingdom  <b>EU entity/business name</b> Thermo Fisher Scientific Janssen Pharmaceuticaaan 3a 2440 Geel, Belgium
Emergency Telephone Number	For information <b>US</b> call: 001-800-227-6701 / <b>Europe</b> call: +32 14 57 52 11 Emergency Number <b>US</b> :001-201-796-7100 / <b>Europe</b> : +32 14 57 52 99 <b>CHEMTREC</b> Tel. No. <b>US</b> :001-800-424-9300 / <b>Europe</b> :001-703-527-3887
E-mail address	begel.sdsdesk@thermofisher.com
Recommended Use Uses advised against	Laboratory chemicals. No Information available

### SECTION 2. HAZARD IDENTIFICATION

Physical State Solid	Appearance White	Odor No information available
<b>Emergency Overview</b> Flammable solid. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.		

#### Classification of the substance or mixture

Flammable solids.	Category 2
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3

#### Label Elements

## 3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione



## Signal Word

## Warning

## Hazard Statements

H228 - Flammable solid  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation

## Precautionary Statements

## Prevention

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
P240 - Ground and bond container and receiving equipment  
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P264 - Wash face, hands and any exposed skin thoroughly after handling  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear protective gloves/protective clothing/eye protection/face protection

## Response

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P312 - Call a POISON CENTER or doctor if you feel unwell  
P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish  
P362 + P364 - Take off contaminated clothing and wash it before reuse

## Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

## Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

## Physical and Chemical Hazards

Combustible material.

## Health Hazards

Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

## Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil.

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

## SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione	175334-68-6	97

## SECTION 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.

**3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione****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. Get medical attention if symptoms occur.

**Most important symptoms and effects**

None reasonably foreseeable.

**Self-Protection of the First Aider**

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

**Notes to Physician**

Treat symptomatically.

**SECTION 5. FIRE-FIGHTING MEASURES****Suitable Extinguishing Media**

Water spray or fog is preferred; if water not available use dry chemical, CO2 or regular foam.

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

No information available.

**Specific Hazards Arising from the Chemical**

Flammable. Combustible material.

**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.

**SECTION 6. ACCIDENTAL RELEASE MEASURES****Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

**Environmental Precautions**

Should not be released into the environment. See Section 12 for additional Ecological Information.

**Methods for Containment and Clean Up**

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

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

**Storage**

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

## 3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

**Exposure Controls****Engineering Measures**

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	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
PVC				

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.

**Skin and body protection**

Long sleeved clothing

**Respiratory Protection**

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.  
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

**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  
**Recommended Filter type:** Particulates filter conforming to EN 143

**Small scale/Laboratory use**

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended half mask:-** Particle filtering: EN149:2001  
When RPE is used a face piece Fit Test should be conducted

**Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

**Environmental exposure controls**

No information available.

**SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

## 3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione

<b>Appearance</b>	White	
<b>Physical State</b>	Solid	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	No data available	
<b>Melting Point/Range</b>	116 - 118 °C / 240.8 - 244.4 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No information available	
<b>Flash Point</b>	No information available	<b>Method -</b> No information available
<b>Evaporation Rate</b>	Not applicable	Solid
<b>Flammability (solid,gas)</b>	No information available	
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	Not applicable	Solid
<b>Specific Gravity / Density</b>	No data available	
<b>Bulk Density</b>	No data available	
<b>Water Solubility</b>	Insoluble	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	Not applicable	Solid
<b>Explosive Properties</b>	No information available	
<b>Oxidizing Properties</b>	No information available	
<b>Molecular Formula</b>	C16 H23 N3 O S	
<b>Molecular Weight</b>	305.44	

## SECTION 10. STABILITY AND REACTIVITY

<b>Stability</b>	Stable under normal conditions.
<b>Hazardous Reactions</b>	None under normal processing.
<b>Hazardous Polymerization</b>	No information available.
<b>Conditions to Avoid</b>	Keep away from open flames, hot surfaces and sources of ignition. Incompatible products.
<b>Materials to avoid</b>	Strong oxidizing agents. Strong acids. Strong bases.

**Hazardous Decomposition Products** Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Sulfur oxides.

## SECTION 11. TOXICOLOGICAL INFORMATION

<b>Product Information</b>	No acute toxicity information is available for this product
<b>(a) acute toxicity;</b>	
<b>(b) skin corrosion/irritation;</b>	Category 2
<b>(c) serious eye damage/irritation;</b>	Category 2
<b>(d) respiratory or skin sensitization;</b>	
<b>Respiratory</b>	No data available

## 3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione

<b>Skin</b>	No data available
<b>(e) germ cell mutagenicity;</b>	No data available
<b>(f) carcinogenicity;</b>	No data available There are no known carcinogenic chemicals in this product
<b>(g) reproductive toxicity;</b>	No data available
<b>(h) STOT-single exposure;</b>	Category 3
<b>Results / Target organs</b>	Respiratory system
<b>(i) STOT-repeated exposure;</b>	No data available
<b>Target Organs</b>	No information available.
<b>(j) aspiration hazard;</b>	Not applicable Solid
<b>Symptoms / effects, both acute and delayed</b>	No information available

## SECTION 12. ECOLOGICAL INFORMATION

<b>Ecotoxicity effects</b>	Do not empty into drains.
<b>Persistence and Degradability</b>	
<b>Persistence</b>	Insoluble in water.
<b>Bioaccumulative Potential</b>	May have some potential to bioaccumulate
<b>Mobility in soil</b>	Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility
<b>Endocrine Disruptor Information</b>	This product does not contain any known or suspected endocrine disruptors
<b>Persistent Organic Pollutant</b>	This product does not contain any known or suspected substance
<b>Ozone Depletion Potential</b>	This product does not contain any known or suspected substance

## SECTION 13. DISPOSAL CONSIDERATIONS

<b>Waste from Residues/Unused Products</b>	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.
<b>Contaminated Packaging</b>	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 empty container away from heat and sources of ignition.
<b>Other Information</b>	Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

## 3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione

## SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport

UN-No	UN1325
Proper Shipping Name	Flammable solid, organic, n.o.s.
Technical Shipping Name	3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione
Hazard Class	4.1
Packing Group	III

IMDG/IMO

UN-No	UN1325
Proper Shipping Name	Flammable solid, organic, n.o.s.
Technical Shipping Name	3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione
Hazard Class	4.1
Packing Group	III

IATA

UN-No	UN1325
Proper Shipping Name	Flammable solid, organic, n.o.s.
Technical Shipping Name	3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione
Hazard Class	4.1
Packing Group	III

Special Precautions for User	No special precautions required
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## SECTION 15. REGULATORY INFORMATION

**International Inventories**

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

**National Regulations**

## SECTION 16. OTHER INFORMATION

Revision Date	01-Sep-2023
Revision Summary	SDS sections updated, 1, 2, 9, 11, 12, 15, 16.

**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.

Legend

CAS - Chemical Abstracts Service

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

EINECS/ELINCS - European Inventory of Existing Commercial Chemical

**3-[4-(tert-Butyl)phenyl]-4-(3-methoxypropyl)-4,5-dihydro-1H-1,2,4-triazole-5-thione**

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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

**DSL/NDL** - 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

**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**