

Revision Date 01-Sep-2023 Revision Number 4

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

1.1. Product identifier

Product Description: 5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

Cat No. : SPB07148DA; SPB07148EA; SPB07148ZZ

Molecular Formula C14 H8 CI F3 N4 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

Thermo Fisher Scientific (Heysham), Shore Road.

Port of Heysham Industrial Park, Heysham, Lancashire, LA3 2XY

United Kingdom

EU entity/business name Thermo Fisher Scientific Janssen Pharmaceuticalaan 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 - Regulation (EC) No 1272/2008

Physical hazards

Flammable solids Category 2 (H228)

Health hazards

Acute oral toxicity Category 4 (H302)

5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

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Acute dermal toxicity
Acute Inhalation Toxicity - Dusts and Mists

Category 4 (H312) Category 4 (H332)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Warning

Hazard Statements

H228 - Flammable solid

H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

Precautionary Statements

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting

P312 - Call a POISON CENTER or doctor if you feel unwell

P280 - Wear protective gloves/protective clothing

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

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

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 - Regulation (EC) No 1272/2008
5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)p	306936-75-4		97	Acute Tox. 4 (H302)
henyl]-4H-1,2,4-triazole-3-thiol				Acute Tox. 4 (H312)
				Acute Tox. 4 (H332)
				Flam. Sol. 2 (H228)

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

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. Get medical attention if

symptoms occur.

Inhalation Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if

symptoms occur.

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.

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

None reasonably foreseeable.

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. Chemical foam.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

Flammable. Combustible material.

Hazardous Combustion Products

Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂), Sulfur oxides, Gaseous hydrogen fluoride (HF), Fluorine, Hydrogen chloride gas.

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

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

6.2. Environmental precautions

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

6.3. Methods and material for containment and cleaning up

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

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

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.

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

Technical Rules for Hazardous Substances (TRGS) 510 Class 4.1B 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

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

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Predicted No Effect Concentration (PNEC)

No information available.

8.2. Exposure controls

Engineering Measures

Use explosion-proof electrical/ventilating/lighting equipment.

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)

5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

Hand Protection Protective gloves

Glove material Breakthrough time Glove thickness Nitrile rubber See manufacturers - Neoprene recommendations Natural rubber PVC	EU standard EN 374	Glove comments (minimum requirement)
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Long sleeved clothing. Skin and body protection

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 compatability, 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 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

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure Small scale/Laboratory use

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

Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State Solid

Appearance No information available No information available Odor **Odor Threshold** No data available

5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

Melting Point/Range 237 - 239 °C / 458.6 - 462.2 °F

Softening Point No data available
Boiling Point/Range No information available

Flammability (liquid) Not applicable Solid

Flammability (solid,gas) No information available

Explosion Limits No data available

Flash Point No information available Method - No information available

Autoignition Temperature

Decomposition Temperature

PH

No data available

No data available

No data available

Viscosity Not applicable Solid

Water Solubility Insoluble

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Vapor Pressure

Density / Specific Gravity

Bulk Density

No data available

No data available

No data available

Vapor Density Not applicable Solid

Particle characteristics No data available

9.2. Other information

Evaporation Rate

Molecular Formula C14 H8 CI F3 N4 S

Molecular Weight 356.76

Flammable solids Burning rate or burning time = > 2.2 mm/s or < 45 secs

Wetted zone passed - No Not applicable - Solid

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 PolymerizationNo information available.Hazardous ReactionsNone under normal processing.

10.4. Conditions to avoid

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

10.5. Incompatible materials

Strong oxidizing agents. Strong reducing agents.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO₂). Sulfur oxides.

Gaseous hydrogen fluoride (HF). Fluorine. Hydrogen chloride gas.

SECTION 11: TOXICOLOGICAL INFORMATION

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

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5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

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Product Information

(a) acute toxicity;

Category 4 Oral Category 4 **Dermal** Inhalation Category 4

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;

Respiratory No data available Skin No data available

No data available (e) germ cell mutagenicity;

No data available (f) carcinogenicity;

There are no known carcinogenic chemicals in this product

No data available (g) reproductive toxicity;

No data available (h) STOT-single exposure;

No data available (i) STOT-repeated exposure;

Target Organs No information available.

(j) aspiration hazard; Not applicable

Solid

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

Symptoms / effects,both acute and No information available.

delayed

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 Do not empty into drains.

5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

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12.2. Persistence and degradability

Insoluble in water. **Persistence**

12.3. Bioaccumulative potential May have some potential to bioaccumulate

12.4. Mobility in soil Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water

solubility.

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.

Dispose of this container to hazardous or special waste collection point. Empty containers **Contaminated Packaging**

retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and

empty container away from heat and sources of ignition.

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

application specific.

Other Information 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.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

UN1325 14.1. UN number

14.2. UN proper shipping name Flammable solid, organic, n.o.s.

Technical Shipping Name 5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

14.3. Transport hazard class(es) 4.1 Ш

14.4. Packing group

ADR

14.1. UN number UN1325

14.2. UN proper shipping name Flammable solid, organic, n.o.s.

5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

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5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol **Technical Shipping Name**

14.3. Transport hazard class(es) 4.1 14.4. Packing group III

IATA

UN1325 14.1. UN number

14.2. UN proper shipping name Flammable solid, organic, n.o.s.

Technical Shipping Name 5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

14.3. Transport hazard class(es) Ш 14.4. Packing group

14.5. Environmental hazards No hazards identified

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
5-(6-Chloro-3-pyridyl)-4-[3-(trifluor	306936-75-4	-		-	-	-	-	-	-
omethyl)phenyl]-4H-1,2,4-triazole-									
3-thiol									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
5-(6-Chloro-3-pyridyl)-4-[3-(trifluor omethyl)phenyl]-4H-1,2,4-triazole- 3-thiol		-	-	-	-	-	-	-

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 Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
5-(6-Chloro-3-pyridyl)-4-[3-(trifluoro methyl)phenyl]-4H-1,2,4-triazole-3-t hiol		-	-	<u>-</u>

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
5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,		Not applicable	Not applicable
4-triazole-3-thiol			

5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

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

Not applicable

import of dangerous chemicals

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 = 3 (self classification)

15.2. Chemical safety assessment

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

SECTION 16: OTHER INFORMATION

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

H228 - Flammable solid

H302 - Harmful if swallowed

H312 - Harmful in contact with skin

H332 - Harmful if inhaled

Legend

CAS - Chemical Abstracts Service

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic

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

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Substances List

ENCS - Japanese Existing and New Chemical Substances AICS - Australian Inventory of Chemical Substances

IARC - International Agency for Research on Cancer

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

EC50 - Effective Concentration 50% POW - Partition coefficient Octanol:Water

TWA - Time Weighted Average

LD50 - Lethal Dose 50%

vPvB - very Persistent, very Bioaccumulative

Predicted No Effect Concentration (PNEC)

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

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

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

MARPOL - International Convention for the Prevention of Pollution from Ships

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5-(6-Chloro-3-pyridyl)-4-[3-(trifluoromethyl)phenyl]-4H-1,2,4-triazole-3-thiol

OECD - Organisation for Economic Co-operation and Development **BCF** - Bioconcentration factor

ATE - Acute Toxicity Estimate
VOC - (Volatile Organic Compound)

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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.

Revision Date 01-Sep-2023

Revision Summary SDS sections updated, 1, 2, 9, 11, 12, 15, 16.

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006. COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No. 1907/2006

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