

Creation Date 09-Oct-2015 Revision Date 24-Aug-2023 **Revision Number 4** 

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

1.1. Product identifier

**Product Description:** 3-[(Cyanomethyl)thio]-5-methyl-4,4-dioxo-4,5-dihydro-4lambda~6~-thieno[3,4-c][2,1]b

enzothiazine-1-carbonitrile

KM03866SC Cat No.: Molecular Formula C14H9N3O2S3

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

Recommended Use Laboratory chemicals. No Information available Uses advised against

1.3. Details of the supplier of the safety data sheet

Company

EU entity/business name Thermo Fisher Scientific Janssen Pharmaceuticalaan 3a

2440 Geel, Belgium

UK entity/business name

Thermo Fisher Scientific (Heysham),

Shore Road,

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

United Kingdom

Swiss distributor - Fisher Scientific AG Neuhofstrasse 11. CH 4153 Reinach

Tel: +41 (0) 56 618 41 11

e-mail - infoch@thermofisher.com

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

customers in Switzerland:

Tox Info Suisse Emergency Number: 145 (24hr)

Tox Info Suisse: +41-44 251 51 51 (Emergency number from abroad)

Chemtrec (24h) Toll-Free: 0800 564 402 Chemtrec Local: +41-43 508 20 11 (Zurich)

# **SECTION 2: HAZARDS IDENTIFICATION**

#### 2.1. Classification of the substance or mixture

3-[(Cyanomethyl)thio]-5-methyl-4,4-dioxo-4,5-dihydro-4lambda~6~-thieno[3,4-c][2,1]benzothiazine-1-carbonitrile

Revision Date 24-Aug-2023

### CLP Classification - Regulation (EC) No 1272/2008

# **Physical hazards**

Based on available data, the classification criteria are not met

#### **Health hazards**

Acute oral toxicity
Acute dermal toxicity
Acute Inhalation Toxicity - Dusts and Mists

Category 4 (H302) 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**

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

## **Precautionary Statements**

P280 - Wear protective gloves/protective clothing

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

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

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

### 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
Maybridge Screening Products: Harmful	N/A		90-100	Acute Tox. 4 (H302) Acute Tox. 4 (H312)

3-[(Cyanomethyl)thio]-5-methyl-4,4-dioxo-4,5-dihydro-4lambda~6~-thieno[3,4-c][2,1]benzothiazine-1-carbonitrile

Revision Date 24-Aug-2023

		Acute Tox. 4 (H332)

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. 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, alcohol-resistant foam.

# Extinguishing media which must not be used for safety reasons

No information available.

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

Thermal decomposition can lead to release of irritating gases and vapors.

#### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO2), Nitrogen oxides (NOx), 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

3-[(Cyanomethyl)thio]-5-methyl-4,4-dioxo-4,5-dihydro-4lambda~6~-thieno[3,4-c][2,1]benzothiazine-1-carbonitrile

Revision Date 24-Aug-2023

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

Should not be released into the environment.

### 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.

# 7.2. Conditions for safe storage, including any incompatibilities

Keep containers tightly closed in a dry, cool and well-ventilated place.

**Technical Rules for Hazardous Substances (TRGS) 510** Storage Class/LGK 11 **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

3-[(Cyanomethyl)thio]-5-methyl-4,4-dioxo-4,5-dihydro-4lambda~6~-thieno[3,4-c][2,1]benzothiazine-1-carbonitrile

Revision Date 24-Aug-2023

#### **Biological limit values**

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

#### 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

### 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.

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** Wear safety glasses with side shields (or goggles) (European standard - EN 166)

Hand Protection Protective gloves

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

**Skin and body protection** Long sleeved clothing.

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

3-[(Cyanomethyl)thio]-5-methyl-4,4-dioxo-4,5-dihydro-4lambda~6~-thieno[3,4-c][2,1]b enzothiazine-1-carbonitrile

Revision Date 24-Aug-2023

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.

Solid

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** 

Odor No information available

**Odor Threshold** No data available

**Melting Point/Range** No data available Measured

**Softening Point** No data available

**Boiling Point/Range** No information available

Flammability (liquid) Not applicable

Flammability (solid,gas) No information available

**Explosion Limits** No data available

**Flash Point** Not applicable Method - No information available

**Autoignition Temperature** Not applicable No data available **Decomposition Temperature** 

No information available Hq

Not applicable **Viscosity** 

Solid

Water Solubility No information available No information available Solubility in other solvents

Partition Coefficient (n-octanol/water)

No data available **Vapor Pressure Density / Specific Gravity** No data available **Bulk Density** No data available

**Vapor Density** Not applicable Solid Particle characteristics No data available

9.2. Other information

**Molecular Formula** C14H9N3O2S3 **Molecular Weight** 347.43873

**Evaporation Rate** 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 Polymerization** Hazardous polymerization does not occur.

None under normal processing. **Hazardous Reactions** 

3-[(Cyanomethyl)thio]-5-methyl-4,4-dioxo-4,5-dihydro-4lambda~6~-thieno[3,4-c][2,1]b enzothiazine-1-carbonitrile

Revision Date 24-Aug-2023

10.4. Conditions to avoid

Incompatible products. Excess heat. Avoid dust formation.

10.5. Incompatible materials

Strong oxidizing agents.

#### 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO2). Nitrogen oxides (NOx). 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 Category 4
Dermal Category 4
Inhalation Category 4

(b) skin corrosion/irritation; No data available

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

(d) respiratory or skin sensitization;

**Respiratory Skin**No data available
No data available

(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 No information available.

(j) aspiration hazard; Not applicable

Solid

**Symptoms / effects,both acute and** No information available. **delayed** 

11.2. Information on other hazards

3-[(Cyanomethyl)thio]-5-methyl-4,4-dioxo-4,5-dihydro-4lambda~6~-thieno[3,4-c][2,1]b Revision Date 24-Aug-2023 enzothiazine-1-carbonitrile

**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** Contains no substances known to be hazardous to the environment or that are not

degradable in waste water treatment plants.

12.2. Persistence and degradability No information available

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** 

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.

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 empty into drains.

**Switzerland - Waste Ordinance** Disposal should be in accordance with applicable regional, national and local laws and

regulations. Ordinance on the Avoidance and the Disposal of Waste (Waste Ordinance,

ADWO) SR 814.600

https://www.fedlex.admin.ch/eli/cc/2015/891/en

# **SECTION 14: TRANSPORT INFORMATION**

3-[(Cyanomethyl)thio]-5-methyl-4,4-dioxo-4,5-dihydro-4lambda~6~-thieno[3,4-c][2,1]benzothiazine-1-carbonitrile

Revision Date 24-Aug-2023

IMDG/IMO Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

ADR Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

<u>IATA</u> Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

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
Maybridge Screening Products:	N/A	-	-	-	-	-	-	-	-
Harmful									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Maybridge Screening Products:  Harmful	N/A	-	-	-	-	-	-	-

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)
Maybridge Screening Products: Harmful	N/A	-	-	-

3-[(Cyanomethyl)thio]-5-methyl-4,4-dioxo-4,5-dihydro-4lambda~6~-thieno[3,4-c][2,1]b enzothiazine-1-carbonitrile

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Repor		
		Notification	Requirements		
Maybridge Screening	N/A	Not applicable	Not applicable		
Products: Harmful					

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

### **Swiss Regulations**

Article 4 para. 4 of the Ordinance on the protection of young people in the workplace (SR 822.115) and Article 1 lit. f of the EAER regulation on hazardous work and young people (SR 822.115.2).

Take note on Article 13 Maternity Ordinance (SR 822.111.52) with regards expectant and nursing mothers.

### 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) is not required (< 10 t/y)

# **SECTION 16: OTHER INFORMATION**

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

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

Substances/EU List of Notified Chemical Substances

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

PICCS - Philippines Inventory of Chemicals and Chemical Substances IECSC - Chinese Inventory of Existing Chemical Substances

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

**KECL** - Korean Existing and Evaluated 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 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

Revision Date 24-Aug-2023

3-[(Cyanomethyl)thio]-5-methyl-4,4-dioxo-4,5-dihydro-4lambda~6~-thieno[3,4-c][2,1]b enzothiazine-1-carbonitrile

Revision Date 24-Aug-2023

PBT - Persistent, Bioaccumulative, Toxic

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

Shins

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** 09-Oct-2015 **Revision Date** 24-Aug-2023

**Revision Summary** 1, 2, 9, SDS sections updated, 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

For Switzerland - Compiled in accordance with the technical provisions referred to in Annex 2, Number 3, ChemO (SR 813.11 - Ordinance on Protection against Dangerous Substances and Preparations).

#### 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**