

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

### 1.1. Product identifier

**Product Description:** 4-Cyano-3-(4-methoxyphenyl)-5-(methylthio)thiophene-2-carboxylic acid  
**Cat No. :** KM02613CB; KM02613DA; KM02613FL; KM02613SC; KM02613ZZ  
**Molecular Formula** C14 H11 N O3 S2

### 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

**EU entity/business name**  
 Thermo Fisher Scientific  
 Janssen Pharmaceuticaaan 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

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

### Physical hazards

Based on available data, the classification criteria are not met

### Health hazards

Acute oral toxicity

Category 4 (H302)

Acute dermal toxicity

Category 4 (H312)

Acute Inhalation Toxicity - Dusts and Mists

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

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

## 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
4-Cyano-3-(4-methoxyphenyl)-5-(methylthio)thiophene-2-carboxylic acid	116493-07-3		97	Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332)

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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. Get medical attention if symptoms occur.
<b>Inhalation</b>	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
<b>Self-Protection of the First Aider</b>	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

<b>Notes to Physician</b>	Treat symptomatically.
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## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### Suitable Extinguishing Media

Water spray. Carbon dioxide (CO<sub>2</sub>). 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

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

#### Hazardous Combustion Products

Nitrogen oxides (NO<sub>x</sub>), 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.

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## 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. 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 at temperature not exceeding 25°C.

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

Storage Class/LGK 11

**Switzerland - Storage of hazardous substances**

Storage class - SC 11/13  
<https://www.kvu.ch/de/themen/stoffe-und-produkte>  
<https://www.kvu.ch/fr/themes/substances-et-produits>  
<https://www.kvu.ch/it/temi/sostanze-e-prodotti>

### 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

## 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

Goggles (European standard - EN 166)

#### Hand Protection

Protective gloves

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

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<b>Large scale/emergency use</b>	Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced <b>Recommended Filter type:</b> Particulates filter conforming to EN 143
<b>Small scale/Laboratory use</b>	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. <b>Recommended half mask:-</b> Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141 When RPE is used a face piece Fit Test should be conducted
<b>Environmental exposure controls</b>	No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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

<b>Physical State</b>	Solid	
<b>Appearance</b>	Light cream	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>Melting Point/Range</b>	209 - 214 °C / 408.2 - 417.2 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No information available	
<b>Flammability (liquid)</b>	Not applicable	Solid
<b>Flammability (solid,gas)</b>	No information available	
<b>Explosion Limits</b>	No data available	
<b>Flash Point</b>	No information available	<b>Method -</b> No information available
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	No data available	
<b>Viscosity</b>	Not applicable	Solid
<b>Water Solubility</b>	Insoluble	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Vapor Pressure</b>	No data available	
<b>Density / Specific Gravity</b>	No data available	
<b>Bulk Density</b>	No data available	
<b>Vapor Density</b>	Not applicable	Solid
<b>Particle characteristics</b>	No data available	

### 9.2. Other information

<b>Molecular Formula</b>	C14 H11 N O3 S2
<b>Molecular Weight</b>	305.38
<b>Evaporation Rate</b>	Not applicable - Solid

## SECTION 10: STABILITY AND REACTIVITY

<b>10.1. Reactivity</b>	None known, based on information available
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<b>10.2. Chemical stability</b>	Stable under normal conditions.
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### 10.3. Possibility of hazardous reactions

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

## 10.4. Conditions to avoid

Incompatible products.

## 10.5. Incompatible materials

Strong oxidizing agents.

## 10.6. Hazardous decomposition products

Nitrogen oxides (NOx). 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	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	No data available
Skin	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

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

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

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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

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

#### Persistence

Insoluble in water.

### 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.

#### 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

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,



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ADWO) SR 814.600  
<https://www.fedlex.admin.ch/eli/cc/2015/891/en>

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

**14.1. UN number** UN3439  
**14.2. UN proper shipping name** NITRILES, SOLID, TOXIC, N.O.S.  
**14.3. Transport hazard class(es)** 6.1  
**14.4. Packing group** III

### ADR

**14.1. UN number** UN3439  
**14.2. UN proper shipping name** NITRILES, SOLID, TOXIC, N.O.S.  
**14.3. Transport hazard class(es)** 6.1  
**14.4. Packing group** III

### IATA

**14.1. UN number** UN3439  
**14.2. UN proper shipping name** NITRILES, SOLID, TOXIC, N.O.S.  
**14.3. Transport hazard class(es)** 6.1  
**14.4. Packing group** III

**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
4-Cyano-3-(4-methoxyphenyl)-5-(methylthio)thiophene-2-carboxylic acid	116493-07-3	-	-	-	-	-	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
4-Cyano-3-(4-methoxyphenyl)-5-(methylthio)thiophene-2-carboxylic acid	116493-07-3	-	-	-	-	-	-	-

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

MAYKM02613

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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)
4-Cyano-3-(4-methoxyphenyl)-5-(methylthio)thiophene-2-carboxylic acid	116493-07-3	-	-	-

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
4-Cyano-3-(4-methoxyphenyl)-5-(methylthio)thiophene-2-carboxylic acid	116493-07-3	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 = 3 (self classification)

## 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) has not been conducted

## 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

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

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

**DSL/NDL** - Canadian Domestic Substances List/Non-Domestic Substances List

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**PICCS** - Philippines Inventory of Chemicals and Chemical Substances  
**IECSC** - Chinese Inventory of Existing Chemical Substances  
**KECL** - Korean Existing and Evaluated Chemical Substances

**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.

Revision Date 24-Aug-2023

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

**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**