

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: Methyl 3-({ 2-cyano-3-[(ethoxycarbonyl)amino]-3-oxoprop-1-enyl} amino)thiophene-2-carboxylate
Cat No. : KM07961SC
Molecular Formula C13H13N3O5S

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 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 - Regulation (EC) No 1272/2008

Physical hazards

Based on available data, the classification criteria are not met

Health hazards

SAFETY DATA SHEET

Methyl 3-((2-cyano-3-[(ethoxycarbonyl)amino]-3-oxoprop-1-enyl)amino)thiophene-2-carboxylate

Revision Date 24-Aug-2023

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) Acute Tox. 4 (H332) |

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

SAFETY DATA SHEET

Methyl 3-({ 2-cyano-3-[(ethoxycarbonyl)amino]-3-oxoprop-1-enyl}
amino)thiophene-2-carboxylate

Revision Date 24-Aug-2023

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 (NO_x), 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

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

6.2. Environmental precautions

SAFETY DATA SHEET

Methyl 3-({ 2-cyano-3-[(ethoxycarbonyl)amino]-3-oxoprop-1-enyl}
amino)thiophene-2-carboxylate

Revision Date 24-Aug-2023

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 Class 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

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.

SAFETY DATA SHEET

Methyl 3-((2-cyano-3-[(ethoxycarbonyl)amino]-3-oxoprop-1-enyl)amino)thiophene-2-carboxylate

Revision Date 24-Aug-2023

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

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

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

Solid

Flammability (solid,gas)

No information available

Explosion Limits

No data available

SAFETY DATA SHEET

Methyl 3-((2-cyano-3-[(ethoxycarbonyl)amino]-3-oxoprop-1-enyl)amino)thiophene-2-carboxylate

Revision Date 24-Aug-2023

| | | |
|---|--------------------------|-----------------------------------|
| Flash Point | Not applicable | Method - No information available |
| Autoignition Temperature | Not applicable | |
| Decomposition Temperature | No data available | |
| pH | No information available | |
| Viscosity | Not applicable | Solid |
| Water Solubility | No information available | |
| Solubility in other solvents | No information available | |
| Partition Coefficient (n-octanol/water) | | |
| Vapor Pressure | No data available | |
| 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 | C13H13N3O5S |
| Molecular Weight | 323.32966 |
| 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. |
| Hazardous Reactions | None under normal processing. |

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 (NO_x). 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 |

SAFETY DATA SHEET

Methyl 3-({ 2-cyano-3-[(ethoxycarbonyl)amino]-3-oxoprop-1-enyl}
amino)thiophene-2-carboxylate

Revision Date 24-Aug-2023

| | |
|--|---|
| (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 |
| Symptoms / effects, both acute and delayed | No information available. |

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 No information available

12.3. Bioaccumulative potential No information available

12.4. Mobility in soil No information available

SAFETY DATA SHEET

Methyl 3-((2-cyano-3-[(ethoxycarbonyl)amino]-3-oxoprop-1-enyl)amino)thiophene-2-carboxylate

Revision Date 24-Aug-2023

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.

SECTION 14: TRANSPORT INFORMATION

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

IATA

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

SAFETY DATA SHEET

Methyl 3-((2-cyano-3-[(ethoxycarbonyl)amino]-3-oxoprop-1-enyl)amino)thiophene-2-carboxylate

Revision Date 24-Aug-2023

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: Harmful | N/A | - | - | - | - | - | - | - | - |

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

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

SAFETY DATA SHEET

Methyl 3-({ 2-cyano-3-[(ethoxycarbonyl)amino]-3-oxoprop-1-enyl}
amino)thiophene-2-carboxylate

Revision Date 24-Aug-2023

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

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

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

**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**

SAFETY DATA SHEET

Methyl 3-({ 2-cyano-3-[(ethoxycarbonyl)amino]-3-oxoprop-1-enyl}
amino)thiophene-2-carboxylate

Revision Date 24-Aug-2023

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