

Revision Date 05-Sep-2023

Revision Number 6

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

1.1. Product identifier

 Product Description:
 5-Methylisoxazole-3-carbonyl chloride

 Cat No. :
 CC10402DA; CC10402EA; CC10402ZZ

 Molecular Formula
 C5 H4 Cl N O2

 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

Based on available data, the classification criteria are not met

Health hazards

Skin Corrosion/Irritation

Category 1 B (H314)

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Serious Eye Damage/Eye Irritation

Category 1 (H318)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Danger

Hazard Statements

Signal Word

H314 - Causes severe skin burns and eye damage EUH014 - Reacts violently with water EUH029 - Contact with water liberates toxic gas

Precautionary Statements

P280 - Wear protective gloves/protective clothing/eye protection/face protection
P301 + P330 + P331 - IF SWALLOWED: Rinse mouth. Do NOT induce vomiting
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P310 - Immediately call a POISON CENTER or doctor/physician
P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

2.3. Other hazards

Decomposes in contact with water

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-Methylisoxazole-3-carbonyl chloride	39499-34-8	EEC No. 254-475-6	> 97	Skin Corr. 1B (H314) (EUH014) (EUH029)

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

General Advice	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Call a physician immediately.
Ingestion	Do NOT induce vomiting. Clean mouth with water. Never give anything by mouth to an unconscious person. Call a physician immediately.
Inhalation	If not breathing, give artificial respiration. Remove from exposure, lie down. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Call a physician immediately.
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
	Causes burns by all exposure routes. Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue

4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician

Treat symptomatically.

and danger of perforation

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Carbon dioxide (CO₂). Dry chemical. Chemical foam. CO₂, dry chemical, dry sand, alcohol-resistant foam.

Extinguishing media which must not be used for safety reasons Contact with water liberates toxic gas. Water.

5.2. Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes. Contact with water liberates toxic gas. Reacts violently with water.

Hazardous Combustion Products

Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂), Chlorine, Hydrogen cyanide (hydrocyanic acid), 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. Thermal decomposition can lead to release of irritating gases and vapors.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation. Use personal protective equipment as required. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

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

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Do not expose spill to water.

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

Do not get in eyes, on skin, or on clothing. Wear personal protective equipment/face protection. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Do not allow contact with water.

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 from any possible contact with water. Corrosives area. Keep under nitrogen. Keep away from water or moist air. Keep containers tightly closed in a dry, cool and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510Class 8AStorage 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

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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

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

Hand Protection

Ensure adequate ventilation, especially in confined areas. 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)

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers	-	EN 374	(minimum requirement)
Butyl rubber	recommendations			
Nitrile rubber				
Neoprene				
PVC				
kin and body prote	ection Long sle	eved 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 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 Acid gases filter Type E Yellow conforming to EN14387
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.

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Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

SAFETY DATA SHEET

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance Odor	No information available No information available	
Odor Threshold	No data available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	104 - 107 °C / 219.2 - 224.6 °F	@ 15 mmHg
Flammability (liquid)	No data available	C To think ig
Flammability (solid,gas)	Not applicable	Liguid
Explosion Limits	No data available	1
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Flash Point	No information available	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
рН	No data available	
Viscosity	No data available	
Water Solubility	Decomposes in contact with water	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/wat		
Vapor Pressure	No data available	
Density / Specific Gravity	No data available	
Bulk Density	Not applicable	Liquid
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	
9.2. Other information		

C5 H4 CI N O2

145.54

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity	Yes
10.2. Chemical stability	Stable under normal conditions. Moisture sensitive.
10.3. Possibility of hazardous reacti	ons_
Hazardous Polymerization Hazardous Reactions	No information available. None under normal processing. Reacts violently with water.
10.4. Conditions to avoid	Incompatible products. Exposure to moist air or water. Exposure to moisture.

Molecular Formula Molecular Weight

10.5. Incompatible materials

Bases. Water. Strong acids. Strong bases. Alcohols. Amines. Acid chlorides. Reducing Agent.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO₂). Chlorine. Hydrogen cyanide (hydrocyanic acid). Hydrogen chloride gas.

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product Information	No acute toxicity information is available for this product
(a) acute toxicity; Oral Dermal Inhalation	No data available No data available No data available
(b) skin corrosion/irritation;	Category 1 B
(c) serious eye damage/irritation;	Category 1
(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;	No data available
Other Adverse Effects	The toxicological properties have not been fully investigated.
Symptoms / effects,both acute and delayed	Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated. Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation.

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

<u>12.1. Toxicity</u> Ecotoxicity effects	Reacts with water so no ecotoxicity data for the substance is available.				
<u>12.2. Persistence and degradability</u> Persistence Degradability Degradation in sewage treatment plant	No information available Persistence is unlikely, based on information available. Decomposes in contact with water. Decomposes in contact with water.				
12.3. Bioaccumulative potential	Product does not bioaccumulate due to reaction with water				
<u>12.4. Mobility in soil</u>	Decomposes in contact with water Is not likely mobile in the environment.				
12.5. Results of PBT and vPvB assessment	Decomposes in contact with water.				
<u>12.6. Endocrine disrupting</u> properties Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors				
<u>12.7. Other adverse effects</u> 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				
SE	CTION 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 produ was used. Do not empty into drains. Do not flush to sewer. Large amounts will affect pH and harm aquatic organisms.				

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

<u>14.1. UN number</u> <u>14.2. UN proper shipping name</u> Technical Shipping Name <u>14.3. Transport hazard class(es)</u> 14.4. Packing group	UN3261 Corrosive solid, acidic, organic, n.o.s. 5-Methylisoxazole-3-carbonyl chloride 8 II
ADR	
<u>14.1. UN number</u> <u>14.2. UN proper shipping name</u> Technical Shipping Name <u>14.3. Transport hazard class(es)</u> <u>14.4. Packing group</u>	UN3261 Corrosive solid, acidic, organic, n.o.s. 5-Methylisoxazole-3-carbonyl chloride 8 II
IATA	
<u>14.1. UN number</u> <u>14.2. UN proper shipping name</u> Technical Shipping Name <u>14.3. Transport hazard class(es)</u> <u>14.4. Packing group</u>	UN3261 Corrosive solid, acidic, organic, n.o.s. 5-Methylisoxazole-3-carbonyl chloride 8 II
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-Methylisoxazole-3-carbonyl chloride	39499-34-8	254-475-6	-	-	-	-	-	-	-
Component	CAS No	TSCA	notific	iventory ation - Inactive	DSL	NDSL	AICS	NZIoC	PICCS
5-Methylisoxazole-3-carbonyl	39499-34-8	-		-	-	-	-	-	-

Legend: X - Listed '-' - Not Listed

chloride

KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

Authorisation/Restrictions according to EU REACH

Not applicable

ſ	Component	CAS No	REACH (1907/2006) -	REACH (1907/2006) -	REACH Regulation (EC
	-		Annex XIV - Substances	Annex XVII - Restrictions	1907/2006) article 59 -
			Subject to Authorization	on Certain Dangerous	Candidate List of
				Substances	Substances of Very High

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				Concern (SVHC)
5-Methylisoxazole-3-carbonyl	39499-34-8	-	-	-
chloride				

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-Methylisoxazole-3-carbony I chloride	39499-34-8	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)

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

H314 - Causes severe skin burns and eye damage

H318 - Causes serious eye damage

EUH014 - Reacts violently with water

EUH029 - Contact with water liberates toxic gas

Legend

CAS - Chemical Abstracts ServiceTSCA - United States Toxic Substances Control Act Section 8(b)
InventoryEINECS/ELINCS - European Inventory of Existing Commercial Chemical
Substances/EU List of Notified Chemical SubstancesDSL/NDSL - Canadian Domestic Substances List/Non-Domestic
Substances ListPICCS - Philippines Inventory of Chemicals and Chemical SubstancesENCS - Japanese Existing and New Chemical Substances
AICS - Australian Inventory of Chemical SubstancesKECL - Korean Existing and Evaluated Chemical SubstancesNZIOC - New Zealand Inventory of Chemicals

5-Methylisoxazole-3-carbonyl chloride

WEL - Workplace Exposure Limit	TWA - Time Weighted Average
ACGIH - American Conference of Governmental Industrial Hygienists	IARC - International Agency for Research on Cancer
DNEL - Derived No Effect Level	Predicted No Effect Concentration (PNEC)
RPE - Respiratory Protective Equipment	LD50 - Lethal Dose 50%
LC50 - Lethal Concentration 50%	EC50 - Effective Concentration 50%
NOEC - No Observed Effect Concentration	POW - Partition coefficient Octanol:Water
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 Key literature references and sources for data https://echa.europa.eu/information-on-chemicals	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)

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	05-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