

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

### 1.1. Product identifier

**Product Description:** 1-[3-(4-Chlorophenyl)-5-methylisoxazol-4-yl]ethan-1-one  
**Cat No. :** SPB04957DA; SPB04957EA; SPB04957EB; SPB04957SC; SPB04957ZZ  
**Molecular Formula** C12 H10 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 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**

Based on available data, the classification criteria are not met

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## Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## 2.2. Label elements

None required

## 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
1-[3-(4-Chlorophenyl)-5-methylisoxazol-4-yl]ethan-1-one	169814-48-6		97	-

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

<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. Get medical attention immediately if symptoms occur.
<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. Get medical attention immediately if symptoms occur.
<b>Self-Protection of the First Aider</b>	No special precautions required.

### 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

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Notes to Physician

Treat symptomatically.

## 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>), 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.

## 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. Avoid dust formation.

### 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. Avoid contact with skin, eyes or 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

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

**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.

### 8.2. Exposure controls

#### **Engineering Measures**

None under normal use conditions.

#### **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 recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

**Skin and body protection**      Wear appropriate protective gloves and clothing to prevent skin exposure.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.

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(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** No protective equipment is needed under normal use conditions.

**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:** Particle filter

**Small scale/Laboratory use** Maintain adequate ventilation

**Environmental exposure controls** 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>	White	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>Melting Point/Range</b>	56 - 59 °C / 132.8 - 138.2 °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>	C12 H10 Cl N O2
<b>Molecular Weight</b>	235.67
<b>Evaporation Rate</b>	Not applicable - Solid

## SECTION 10: STABILITY AND REACTIVITY

**10.1. Reactivity** None known, based on information available

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## 10.2. Chemical stability

Stable under normal conditions.

## 10.3. Possibility of hazardous reactions

**Hazardous Polymerization**  
**Hazardous Reactions**

No information available.  
None under normal processing.

## 10.4. Conditions to avoid

Incompatible products.

## 10.5. Incompatible materials

Bases. Amines. Reducing Agent.

## 10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). 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**

No data available

**Dermal**

No data available

**Inhalation**

No data available

**(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.

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(j) aspiration hazard; Not applicable  
Solid

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

**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

**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** This product does not contain any known or suspected substance  
**Ozone Depletion Potential** This product does not contain any known or suspected substance

## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

**Waste from Residues/Unused Products** Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

**Contaminated Packaging** Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers.

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**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.

## 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

**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
1-[3-(4-Chlorophenyl)-5-methylisoxazol-4-yl]ethan-1-one	169814-48-6	-	-	-	-	-	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
1-[3-(4-Chlorophenyl)-5-methylisoxazol-4-yl]ethan-1-one	169814-48-6	-	-	-	-	-	-	-



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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)
1-[3-(4-Chlorophenyl)-5-methylisoxazol-4-yl]ethan-1-one	169814-48-6	-	-	-

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
1-[3-(4-Chlorophenyl)-5-methylisoxazol-4-yl]ethan-1-one	169814-48-6	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

### Legend

CAS - Chemical Abstracts Service

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

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

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.

**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**