

according to Regulation UK SI 2019/758 and UK SI 2020/1577 as amended

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: 1-benzyl-2-(methylsulfanyl)-1H-imidazole-5-carbonyl chloride hydrochloride

Cat No.: CC28902CB; CC28902DA; CC28902DE; CC28902ZZ

Molecular Formula C12 H11 CI N2 O S . H CI

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

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Acute oral toxicity

Acute dermal toxicity

Acute Inhalation Toxicity - Dusts and Mists

Category 4 (H302)

Category 4 (H312)

Category 4 (H332)

Category 4 (H332)

Skin Corrosion/Irritation Category 1 B (H314)
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



Signal Word

Danger

Hazard Statements

H314 - Causes severe skin burns and eye damage

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

EUH014 - Reacts violently with water

EUH029 - Contact with water liberates toxic gas

Precautionary Statements

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

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
1-benzyl-2-(methylsulfanyl)-1H-imidazole-5 -carbonyl chloride hydrochloride	568577-86-6		> 97	Skin Corr. 1B (H314) Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332) (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. Keep eye wide open while rinsing.

Skin Contact Wash off immediately with soap and plenty of water while removing all contaminated

clothes and shoes. Call a physician immediately.

Immediate medical attention is required. Do NOT induce vomiting. Drink plenty of water.

Never give anything by mouth to an unconscious person.

Inhalation Remove to fresh air. If not breathing, give artificial respiration. Call a physician or poison

control center immediately. 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.

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 and danger of perforation

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

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

The product causes burns of eyes, skin and mucous membranes. Contact with water liberates toxic gas. Reacts violently with water.

Hazardous Combustion Products

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

Use personal protective equipment as required. Evacuate personnel to safe areas. Avoid contact with skin, eyes or clothing.

6.2. Environmental precautions

Should not be released into the environment. Do not allow material to contaminate ground water system. 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. 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 dust. 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) 510 Class 8A Storage Class (LGK) (Germany)

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

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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

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)

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 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

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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 White

Odor No information available
Odor Threshold No data available

Melting Point/Range 115 - 122 °C / 239 - 251.6 °F

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

Flash Point No information available Method - No information available

Autoignition Temperature
Decomposition Temperature
PH
No data available
No data available
No data available

Viscosity Not applicable Solid

Water Solubility Decomposes in contact with water

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Vapor Pressure

Density / Specific Gravity

Bulk Density

No data available
No data available
No data available
No data available

Vapor Density Not applicable Solid

Particle characteristics No data available

9.2. Other information

Molecular Formula C12 H11 CI N2 O S . H CI

Molecular Weight 303.21

Evaporation Rate Not applicable - Solid

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity Yes

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous Polymerization No information available.

Hazardous Reactions None under normal processing. Reacts violently with water.

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10.4. Conditions to avoid

Incompatible products, Exposure to moist air or water, Exposure to moisture.

10.5. Incompatible materials

Water. Strong oxidizing agents. Strong bases. Amines.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO2). Sulfur oxides. Hydrogen chloride gas.

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; Category 1 B

(c) serious eye damage/irritation; Category 1

(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

No data available (h) STOT-single exposure;

No data available (i) STOT-repeated exposure;

No information available. **Target Organs**

Not applicable (j) aspiration hazard;

Solid

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

delayed

Symptoms / effects,both acute and 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.

1-benzyl-2-(methylsulfanyl)-1H-imidazole-5-carbonyl chloride hydrochloride

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 Reacts with water so no ecotoxicity data for the substance is available.

12.2. Persistence and degradability No information available

Persistence is unlikely, based on information available. **Persistence**

Degradability Decomposes in contact with water. Degradation in sewage Decomposes in contact with water.

treatment plant

12.3. Bioaccumulative potential Product does not bioaccumulate due to reaction with water

12.4. Mobility in soil Decomposes in contact with water Is not likely mobile in the environment.

12.5. Results of PBT and vPvB Decomposes in contact with water.

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 Waste is classified as hazardous. Dispose of in accordance with the European Directives **Products**

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. Do not flush to sewer. Large amounts will affect pH

and harm aquatic organisms.

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SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN3261

14.2. UN proper shipping name Corrosive solid, acidic, organic, n.o.s.

1-benzyl-2-(methylsulfanyl)-1H-imidazole-5-carbonyl chloride hydrochloride

1-benzyl-2-(methylsulfanyl)-1H-imidazole-5-carbonyl chloride hydrochloride **Technical Shipping Name**

14.3. Transport hazard class(es) 14.4. Packing group II

ADR

14.1. UN number UN3261

14.2. UN proper shipping name Corrosive solid, acidic, organic, n.o.s.

Technical Shipping Name 1-benzyl-2-(methylsulfanyl)-1H-imidazole-5-carbonyl chloride hydrochloride

14.3. Transport hazard class(es) 14.4. Packing group П

IATA

UN3261 14.1. UN number

Corrosive solid, acidic, organic, n.o.s. 14.2. UN proper shipping name

Technical Shipping Name 1-benzyl-2-(methylsulfanyl)-1H-imidazole-5-carbonyl chloride hydrochloride

14.3. Transport hazard class(es) 14.4. Packing group II

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk Not applicable, packaged goods according to IMO instruments

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-benzyl-2-(methylsulfanyl)-1H-imi	568577-86-6	-	-	-	-	-	-	-	-
dazole-5-carbonyl chloride									
hydrochloride									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
1-benzyl-2-(methylsulfanyl)-1H-imi	568577-86-6	-	=	-	-	-	-	-
dazole-5-carbonyl chloride								
hydrochloride								

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

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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)
1-benzyl-2-(methylsulfanyl)-1H-imid azole-5-carbonyl chloride hydrochloride	568577-86-6	-	-	-

Seveso III Directive (2012/18/EC)

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-benzyl-2-(methylsulfanyl)- 1H-imidazole-5-carbonyl chloride hydrochloride	568577-86-6	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

EUH014 - Reacts violently with water

EUH029 - Contact with water liberates toxic gas

H302 - Harmful if swallowed

H312 - Harmful in contact with skin

H332 - Harmful if inhaled

H314 - Causes severe skin burns and eye damage

H318 - Causes serious eye damage

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Legend

CAS - Chemical Abstracts Service

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

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

Substances List

PICCS - Philippines Inventory of Chemicals and Chemical Substances

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

IECSC - Chinese Inventory of Existing 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 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

VOC - (Volatile Organic Compound)

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

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

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.

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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