

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

Creation Date 26-Sep-2009 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: 4-Methyl-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride

Cat No.: CC36103CB; CC36103DA; CC36103ZZ

Molecular Formula C9 H10 O3 N S 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

4-Methyl-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride

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Skin Corrosion/Irritation

Serious Eye Damage/Eye Irritation

Category 1 B (H314) 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

EUH029 - Contact with water liberates toxic gas

EUH014 - Reacts violently with water

Precautionary Statements

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting

P280 - Wear eye protection/ face protection

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

P402 + P404 - Store in a dry place. Store in a closed container

2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	EC No	Weight %	CLP Classification - Regulation (EC) No 1272/2008
4-Methyl-3,4-dihydro-2H-1,4-benzoxazine-6 -sulfonyl chloride	892948-94-6		> 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

4-Methyl-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride

Eve ContactRinse 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. Immediate medical

attention is required.

Ingestion Do NOT induce vomiting. Call a physician or poison control center immediately.

Inhalation Remove to fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial

respiration. 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. Immediate medical attention is required.

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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.

Extinguishing media which must not be used for safety reasons

Water.

5.2. Special hazards arising from the substance or mixture

Contact with water liberates toxic gas. Water reactive. Produce flammable gases on contact with water.

Hazardous Combustion Products

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.

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. Avoid dust formation.

6.2. Environmental precautions

4-Methyl-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride

Prevent further leakage or spillage if safe to do so.

6.3. Methods and material for containment and cleaning up

Sweep up and shovel into suitable containers for disposal. Do not expose spill to water. Do not let this chemical enter the environment. 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

Use only under a chemical fume hood. Wear personal protective equipment/face protection. Do not breathe dust. Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Do not allow contact with water. Do not allow contact with water because of violent reaction. Handle under argon. Minimize dust generation and accumulation. Wash hands before breaks and immediately after handling the product.

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.

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

Class 8B

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

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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
Disposable gloves	See manufacturers	-	EN 374	(minimum requirement)
	recommendations			

Skin and body protectionWear 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. (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 Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard

EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

To protect the wearer, respiratory protective equipment must be the correct fit and be used

and maintained properly

Large scale/emergency use In case of insufficient ventilation, wear suitable respiratory equipment

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.

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 Low melting solid Solid

Appearance Off-white

Odor No information available
Odor Threshold No data available

4-Methyl-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride

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Melting Point/Range 65 - 69 °C / 149 - 156.2 °F

Softening Point No data available
Boiling Point/Range No information available

Flammability (liquid) Not applicable Solid

Flammability (solid,gas)

Explosion Limits

No information available

No data available

Flash Point No information available Method - No information available

Autoignition Temperature
Decomposition Temperature
pH
Viscosity
Water Solubility
Solubility in other solvents
No data available
No data available
No data available
No information available
No information available

Partition Coefficient (n-octanol/water)

Vapor Pressure
Density / Specific Gravity
Bulk Density
Vapor Density
No data available
No data available
No data available
No data available

Particle characteristics No data available

9.2. Other information

Molecular Formula C9 H10 O3 N S CI

Molecular Weight 247.7

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity Yes

10.2. Chemical stability

Water reactive. Contact with water liberates toxic gas.

10.3. Possibility of hazardous reactions

Hazardous PolymerizationNo information available.Hazardous ReactionsNo information available.

10.4. Conditions to avoid

Incompatible products. Exposure to moist air or water. Avoid dust formation.

10.5. Incompatible materials

Water. Strong oxidizing agents. Strong acids. Strong bases. Strong reducing agents. Acid

(Air = 1.0)

chlorides.

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 No acute toxicity information is available for this product

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(a) acute toxicity:

Oral No data available No data available **Dermal** Inhalation No data available

No data available (b) skin corrosion/irritation;

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;

Respiratory No data available No data available Skin

(e) germ cell mutagenicity; No data available

No data available (f) carcinogenicity;

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

No data available (h) STOT-single exposure;

(i) STOT-repeated exposure; No data available

No information available. **Target Organs**

(j) aspiration hazard; No data available

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.

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

Do not empty into drains. **Ecotoxicity effects**

12.2. Persistence and degradability No information available

4-Methyl-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride

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12.3. Bioaccumulative potential No information available

12.4. Mobility in soil No information available

12.5. Results of PBT and vPvB

<u>assessment</u>

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

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.

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

UN3261 14.1. UN number

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

Technical Shipping Name 4-Methyl-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride 14.3. Transport hazard class(es)

14.4. Packing group

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<u>ADR</u>

14.1. UN number UN3261

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

Technical Shipping Name 4-Methyl-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride

14.3. Transport hazard class(es) 8

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14.4. Packing group

IATA

4-Methyl-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride

14.1. UN number UN3261

14.2. UN proper shipping name CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.*

Technical Shipping Name 4-Methyl-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride

14.3. Transport hazard class(es) 8 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 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
4-Methyl-3,4-dihydro-2H-1,4-benz	892948-94-6	-	-	-	-	-	-	-	-
oxazine-6-sulfonyl chloride									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
4-Methyl-3,4-dihydro-2H-1,4-benz oxazine-6-sulfonyl chloride	892948-94-6	-	-	1	-	-	-	-

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 Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
4-Methyl-3,4-dihydro-2H-1,4-benzox azine-6-sulfonyl chloride	892948-94-6	-	-	-

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
4-Methyl-3,4-dihydro-2H-1,4- benzoxazine-6-sulfonyl chloride	892948-94-6	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

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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

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

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

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

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)

NZIoC - New Zealand Inventory of Chemicals

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.

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05-Sep-2023 **Revision Date**

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