

Revision Date 05-Sep-2023

**Revision Number** 4

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

1.1. Product identifier

Product Description: Cat No. : Molecular Formula	3,4-Dihydro-2H-1,5-benzodioxepine-7-sulfonyl chloride CC13203CB; CC13203DA; CC13203ZZ C9 H9 CI O4 S	
1.2. Relevant identified uses of the	substance or mixture and uses advised against	
Recommended Use Uses advised against	Laboratory chemicals. 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 <b>US</b> call: 001-800-227-6701 / <b>Europe</b> call: +32 14 57 52 11	

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)

#### 3,4-Dihydro-2H-1,5-benzodioxepine-7-sulfonyl chloride

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Category 1 (H318)

Serious Eye Damage/Eye Irritation

#### 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

#### **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
3,4-Dihydro-2H-1,5-benzodioxepine-7-sulfo nyl chloride	321309-38-0		97	Skin Corr. 1B (H314)

Full text of Hazard Statements: see section 16

# **SECTION 4: FIRST AID MEASURES**

#### 4.1. Description of first aid measures

3,4-Dihydro-2H-1,5-benzodioxepine-7-sulfonyl chloride

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.	
Ingestion	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 (CO<sub>2</sub>). Dry chemical. Chemical foam. CO<sub>2</sub>, dry chemical, dry sand, 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

The product causes burns of eyes, skin and mucous membranes.

#### Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Fumes, Chlorine, 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.

#### 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.

#### **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. Corrosives area. Store under an inert atmosphere. 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

#### 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)

Protective gloves

Hand Protection

Natur Buty Nitrilo Neo	al rubber See	akthrough time e manufacturers ommendations	Glove thickness	EU standard EN 374	Glove comments (minimum requirement)
Skin ar	nd body protection	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 <b>Recommended Filter type:</b> 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. <b>Recommended half mask:-</b> 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

Environmental exposure controls No information available.

### **SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES**

#### 9.1. Information on basic physical and chemical properties

#### 3,4-Dihydro-2H-1,5-benzodioxepine-7-sulfonyl chloride

Physical State	Solid	
Appearance Odor Odor Threshold Melting Point/Range Softening Point Boiling Point/Range Flammability (liquid) Flammability (solid,gas) Explosion Limits	Off-white No information available No data available 50 - 52 °C / 122 - 125.6 °F No data available No information available No information available No information available No data available	Solid
Flash Point Autoignition Temperature Decomposition Temperature pH	No information available No data available No data available No data available	Method - No information available
Viscosity Water Solubility Solubility in other solvents Partition Coefficient (n-octanol/wat Vapor Pressure	Not applicable Decomposes in contact with water No information available	Solid
Density / Specific Gravity Bulk Density Vapor Density Particle characteristics	No data available No data available Not applicable No data available	Solid
9.2. Other information		
Molecular Formula Molecular Weight Evaporation Rate	C9 H9 Cl O4 S 248.69 Not applicable - Solid	

# **SECTION 10: STABILITY AND REACTIVITY**

10.1. Reactivity	None known, based on information available	
10.2. Chemical stability	Moisture sensitive.	
10.3. Possibility of hazardous react	ions	
Hazardous Polymerization Hazardous Reactions	No information available. None under normal processing.	
10.4. Conditions to avoid	Incompatible products. Exposure to moist air or water.	
10.5. Incompatible materials	Bases. Strong oxidizing agents. Alcohols. Amines.	
10.6. Hazardous decomposition products Carbon monoxide (CO). Carbon dioxide (CO2). Fumes. Chlorine. Sulfur oxides. Hydrogen chloride gas.		

# **SECTION 11: TOXICOLOGICAL INFORMATION**

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

### No acute toxicity information is available for this product **Product Information** (a) acute toxicity; Oral No data available Dermal No data available No data available Inhalation Category 1 B (b) skin corrosion/irritation; (c) serious eye damage/irritation; Category 1 (d) respiratory or skin sensitization; No data available Respiratory Skin No data available (e) germ cell mutagenicity; No data available No data available (f) carcinogenicity; There are no known carcinogenic chemicals in this product No data available (g) reproductive toxicity; 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. Symptoms / effects, both acute and Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. delayed 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 Assess endocrine disrupting properties for human health. This product does not contain any **Endocrine Disrupting Properties** 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 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.
<u>12.5. Results of PBT and vPvB</u> 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
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. 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>	UN3261
<u>14.2. UN proper shipping name</u>	Corrosive solid, acidic, organic, n.o.s.
Technical Shipping Name	3,4-Dihydro-2H-1,5-benzodioxepine-7-sulfonyl chloride
<u>14.3. Transport hazard class(es)</u>	8
14.4. Packing group	III

3,4-Dihydro-2H-1,5-benzodioxepine-7-sulfonyl chloride

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> 14.4. Packing group	UN3261 Corrosive solid, acidic, organic, n.o.s. 3,4-Dihydro-2H-1,5-benzodioxepine-7-sulfonyl chloride 8 III
<u>IATA</u>	
<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. 3,4-Dihydro-2H-1,5-benzodioxepine-7-sulfonyl chloride 8 III
14.5. Environmental hazards	No hazards identified
14.6. Special precautions for user	No special precautions required.
<u>14.7. Maritime transport in bulk</u> 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
3,4-Dihydro-2H-1,5-benzodioxepin	321309-38-0	-	-	-	-	-	-	-	-
e-7-sulfonyl chloride									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
3,4-Dihydro-2H-1,5-benzodioxepin e-7-sulfonyl chloride	321309-38-0	-	-	-	-	-	-	-

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	5	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
3,4-Dihydro-2H-1,5-benzodioxepine -7-sulfonyl chloride	321309-38-0	-	-	-

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
3,4-Dihydro-2H-1,5-benzodi oxepine-7-sulfonyl chloride	321309-38-0	Not applicable	Not applicable

3,4-Dihydro-2H-1,5-benzodioxepine-7-sulfonyl chloride

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

#### Legend

CAS - Chemical Abstracts Service	TSCA - United States Toxic Substances Control Act Section 8(b) Inventory
<b>EINECS/ELINCS</b> - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances <b>PICCS</b> - Philippines Inventory of Chemicals and Chemical Substances <b>IECSC</b> - Chinese Inventory of Existing Chemical Substances <b>KECL</b> - Korean Existing and Evaluated Chemical Substances	
<ul> <li>WEL - Workplace Exposure Limit</li> <li>ACGIH - American Conference of Governmental Industrial Hygienists</li> <li>DNEL - Derived No Effect Level</li> <li>RPE - Respiratory Protective Equipment</li> <li>LC50 - Lethal Concentration 50%</li> <li>NOEC - No Observed Effect Concentration</li> <li>PBT - Persistent, Bioaccumulative, Toxic</li> </ul>	<ul> <li>TWA - Time Weighted Average</li> <li>IARC - International Agency for Research on Cancer</li> <li>Predicted No Effect Concentration (PNEC)</li> <li>LD50 - Lethal Dose 50%</li> <li>EC50 - Effective Concentration 50%</li> <li>POW - Partition coefficient Octanol:Water</li> <li>vPvB - very Persistent, very Bioaccumulative</li> </ul>
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)

#### 3,4-Dihydro-2H-1,5-benzodioxepine-7-sulfonyl chloride

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.

Revision Date05-Sep-2023Revision Summary16, SDS sections updated, 1, 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 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**