

## SAFETY DATA SHEET

Creation Date 27-Sep-2014

Revision Date 05-Sep-2023

Revision Number 2

### 1. Identification

**Product Name** 3-Oxo-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride

**Cat No. :** CC46803CB; CC46803DA; CC46803DE; CC46803ZZ

**Synonyms** No information available

**Recommended Use** Laboratory chemicals.

**Uses advised against** Food, drug, pesticide or biocidal product use.

#### Details of the supplier of the safety data sheet

##### Company

Fisher Scientific Company  
One Reagent Lane  
Fair Lawn, NJ 07410  
Tel: (201) 796-7100

Thermo Fisher Scientific  
One Reagent Lane  
Fair Lawn, NJ 07410

##### **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

### 2. Hazard(s) identification

#### Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Skin Corrosion/Irritation	Category 1 B
Serious Eye Damage/Eye Irritation	Category 1

#### Label Elements

##### **Signal Word**

Danger

##### **Hazard Statements**

Causes severe skin burns and eye damage



**Precautionary Statements**

**Prevention**

Do not breathe dust/fume/gas/mist/vapors/spray  
Wash face, hands and any exposed skin thoroughly after handling  
Wear protective gloves/protective clothing/eye protection/face protection

**Response**

Immediately call a POISON CENTER or doctor/physician

**Inhalation**

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

**Skin**

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower  
Wash contaminated clothing before reuse  
Immediately call a POISON CENTER or doctor/physician

**Eyes**

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
Immediately call a POISON CENTER or doctor/physician

**Ingestion**

IF SWALLOWED: Rinse mouth. DO NOT induce vomiting

**Fire**

In case of fire: Use CO2, dry chemical, or foam for extinction

**Storage**

Store locked up

**Disposal**

Dispose of contents/container to an approved waste disposal plant

**Hazards not otherwise classified (HNOC)**

Reacts violently with water  
Contact with water liberates toxic gas

**3. Composition/Information on Ingredients**

Component	CAS No	Weight %
3-Oxo-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride	31794-45-3	> 97

**4. First-aid measures**

<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Inhalation</b>	Remove from exposure, lie down. Remove to fresh air. If breathing is difficult, give oxygen. 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.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately.

<b>Most important symptoms and effects</b>	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
<b>Notes to Physician</b>	Treat symptomatically

### 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Carbon dioxide (CO <sub>2</sub> ). Dry chemical. Chemical foam.
<b>Unsuitable Extinguishing Media</b>	DO NOT USE WATER OR FOAM
<b>Flash Point</b>	No information available
<b>Method -</b>	No information available
<b>Autoignition Temperature</b>	No information available
<b>Explosion Limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Sensitivity to Mechanical Impact</b>	No information available
<b>Sensitivity to Static Discharge</b>	No information available

**Specific Hazards Arising from the Chemical**  
Contact with water liberates toxic gas. Water reactive.

**Hazardous Combustion Products**  
Nitrogen oxides (NO<sub>x</sub>). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Sulfur oxides. Hydrogen chloride gas.

**Protective Equipment and Precautions for Firefighters**  
As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

<b><u>NFPA</u></b>	<b>Health</b>	<b>Flammability</b>	<b>Instability</b>	<b>Physical hazards</b>
	3	1	0	W

### 6. Accidental release measures

<b>Personal Precautions</b>	Ensure adequate ventilation. Use personal protective equipment as required.
<b>Environmental Precautions</b>	See Section 12 for additional Ecological Information.
<b>Methods for Containment and Clean Up</b>	Wear self-contained breathing apparatus and protective suit. 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. Use spark-proof tools and explosion-proof equipment.

### 7. Handling and storage

<b>Handling</b>	Wear personal protective equipment/face protection. Do not breathe dust. Do not breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Handle product only in closed system or provide appropriate exhaust ventilation. Do not allow contact with water because of violent reaction. Handle under argon.
<b>Storage.</b>	Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Protect from moisture. Keep from any possible contact with water. Corrosives area. Incompatible Materials. Water. Strong oxidizing agents. Strong acids. Strong bases. Amines. Strong reducing agents. Acid chlorides.

## 8. Exposure controls / personal protection

<b>Exposure Guidelines</b>	This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.
<b>Engineering Measures</b>	Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Use spark-proof tools and explosion-proof equipment.
<b>Personal Protective Equipment</b>	
<b>Eye/face Protection</b>	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
<b>Skin and body protection</b>	Wear appropriate protective gloves and clothing to prevent skin exposure.
<b>Respiratory Protection</b>	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.
<b>Hygiene Measures</b>	Handle in accordance with good industrial hygiene and safety practice.

## 9. Physical and chemical properties

<b>Physical State</b>	Solid
<b>Appearance</b>	White
<b>Odor</b>	No information available
<b>Odor Threshold</b>	No information available
<b>pH</b>	No information available
<b>Melting Point/Range</b>	178 °C / 352.4 °F
<b>Boiling Point/Range</b>	No information available
<b>Flash Point</b>	No information available
<b>Evaporation Rate</b>	No information available
<b>Flammability (solid,gas)</b>	No information available
<b>Flammability or explosive limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Vapor Pressure</b>	No information available
<b>Vapor Density</b>	No information available
<b>Specific Gravity</b>	No information available
<b>Solubility</b>	No information available
<b>Partition coefficient; n-octanol/water</b>	No data available
<b>Autoignition Temperature</b>	No information available
<b>Decomposition Temperature</b>	No information available
<b>Viscosity</b>	No information available
<b>Molecular Formula</b>	C8 H6 Cl N O4 S
<b>Molecular Weight</b>	247.66

## 10. Stability and reactivity

<b>Reactive Hazard</b>	Yes
<b>Stability</b>	Stable under normal conditions. Moisture sensitive.
<b>Conditions to Avoid</b>	Incompatible products. Exposure to moist air or water.

**Incompatible Materials** Water, Strong oxidizing agents, Strong acids, Strong bases, Amines, Strong reducing agents, Acid chlorides

**Hazardous Decomposition Products** Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Sulfur oxides, Hydrogen chloride gas

**Hazardous Polymerization** No information available.

**Hazardous Reactions** None under normal processing.

**11. Toxicological information**

**Acute Toxicity**

**Product Information** No acute toxicity information is available for this product

**Component Information**

**Toxicologically Synergistic Products** No information available

**Delayed and immediate effects as well as chronic effects from short and long-term exposure**

**Irritation** No information available

**Sensitization** No information available

**Carcinogenicity** The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
3-Oxo-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride	31794-45-3	Not listed	Not listed	Not listed	Not listed	Not listed

**Mutagenic Effects** No information available

**Reproductive Effects** No information available.

**Developmental Effects** No information available.

**Teratogenicity** No information available.

**STOT - single exposure** None known

**STOT - repeated exposure** None known

**Aspiration hazard** No information available

**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

**Endocrine Disruptor Information** No information available

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

**12. Ecological information**

**Ecotoxicity**

Do not empty into drains.

**Persistence and Degradability** No information available

**Bioaccumulation/ Accumulation** No information available.

**Mobility** No information available.

### 13. Disposal considerations

**Waste Disposal Methods** Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

### 14. Transport information

**DOT**

**UN-No** UN3096  
**Proper Shipping Name** CORROSIVE SOLID, WATER-REACTIVE, N.O.S.  
**Technical Name** (3-OXO-3,4-DIHYDRO-2H-1,4-BENZOXAZINE-6-SULFONYL CHLORIDE)  
**Hazard Class** 8  
**Subsidiary Hazard Class** 4.3  
**Packing Group** II

**TDG**

**UN-No** UN3261  
**Proper Shipping Name** Corrosive solid, acidic, organic, n.o.s.  
**Hazard Class** 8  
**Packing Group** II

**IATA**

**UN-No** UN3261  
**Proper Shipping Name** Corrosive solid, acidic, organic, n.o.s.  
**Hazard Class** 8  
**Packing Group** II

**IMDG/IMO**

**UN-No** UN3261  
**Proper Shipping Name** Corrosive solid, acidic, organic, n.o.s.  
**Hazard Class** 8  
**Packing Group** II

### 15. Regulatory information

**United States of America Inventory**

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
3-Oxo-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride	31794-45-3	-	-	-

**Legend:**

**TSCA** US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

- - Not Listed

**TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)** Not applicable

**TSCA 12(b) - Notices of Export** Not applicable

**International Inventories**

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
3-Oxo-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride	31794-45-3	-	-	-	-	-	-	-	-	-

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

**U.S. Federal Regulations**

**SARA 313** Not applicable

**SARA 311/312 Hazard Categories** See section 2 for more information

**CWA (Clean Water Act)** Not applicable

**Clean Air Act** Not applicable

**OSHA - Occupational Safety and Health Administration** Not applicable

**CERCLA** Not applicable

**California Proposition 65** This product does not contain any Proposition 65 chemicals.

**U.S. State Right-to-Know Regulations** Not applicable

**U.S. Department of Transportation**

Reportable Quantity (RQ): N  
 DOT Marine Pollutant N  
 DOT Severe Marine Pollutant N

**U.S. Department of Homeland Security** This product does not contain any DHS chemicals.

**Other International Regulations**

**Mexico - Grade** No information available

**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)
3-Oxo-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride	31794-45-3	-	-	-

**Safety, health and environmental regulations/legislation specific for the substance or mixture**

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
3-Oxo-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride	31794-45-3	Not applicable	Not applicable	Not applicable	Not applicable

**Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?**  
 Not applicable

**Other International Regulations**

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	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
3-Oxo-3,4-dihydro-2H-1,4-benzoxazine-6-sulfonyl chloride	31794-45-3	Not applicable	Not applicable	Not applicable	Not applicable

## 16. Other information

<b>Prepared By</b>	Regulatory Affairs Thermo Fisher Scientific Email: EMSDS.RA@thermofisher.com
<b>Creation Date</b>	27-Sep-2014
<b>Revision Date</b>	05-Sep-2023
<b>Print Date</b>	05-Sep-2023
<b>Revision Summary</b>	This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

### 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 SDS**