

## Chemical Safety Data Sheet MSDS / SDS

**3-[(2S,4S)-4-Mercaptopyrrolidine-2-carboxamido]benzoic acid hydrochloride**

Revision Date:2024-07-06 Revision Number:1

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 3-[(2S,4S)-4-Mercaptopyrrolidine-2-carboxamido]benzoic acid hydrochloride  
CBnumber : CB1971859  
CAS : 219909-83-8  
EINECS Number : 606-882-9  
Synonyms : 3-[(2S,4S)-4-Mercaptopyrrolidine-2-carboxamido]benzoic acid hydrochloride

**Relevant identified uses of the substance or mixture and uses advised against**

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

**SECTION 2: Hazards identification****Classification of the substance or mixture**

Self- heating substances and mixtures, Category 2  
Skin sensitization, Category 1  
Eye irritation, Category 2  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

**Label elements****Pictogram(s)**

Signal word : Warning

**Hazard statement(s)**

H252 Self-heating in large quantities; may catch fire  
H317 May cause an allergic skin reaction  
H319 Causes serious eye irritation  
H412 Harmful to aquatic life with long lasting effects

**Precautionary statement(s)**

## Prevention

P235 Keep cool.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P272 Contaminated work clothing should not be allowed out of the workplace.

P264 Wash ... thoroughly after handling.

P273 Avoid release to the environment.

## Response

P302+P352 IF ON SKIN: Wash with plenty of water/...

P333+P317 If skin irritation or rash occurs: Get medical help.

P321 Specific treatment (see ... on this label).

P362+P364 Take off contaminated clothing and wash it before reuse.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

## Storage

P407 Maintain air gap between stacks or pallets.

P410 Protect from sunlight.

P413 Store bulk masses greater than ... kg/...lbs at temperatures not exceeding ...°C/...°F.

P420 Store separately.

## Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

## Other hazards

no data available

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# SECTION 3: Composition/information on ingredients

## Substance

Product name	: 3-[(2S,4S)-4-Mercaptopyrrolidine-2-carboxamido]benzoic acid hydrochloride
Synonyms	: 3-[(2S,4S)-4-Mercaptopyrrolidine-2-carboxamido]benzoic acid hydrochloride
CAS	: 219909-83-8
EC number	: 606-882-9
MF	: C <sub>12</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>3</sub> S
MW	: 302.78

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# SECTION 4: First aid measures

## Description of first aid measures

### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately.

Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### **Following skin contact**

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### **Following eye contact**

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### **Following ingestion**

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

#### **Most important symptoms and effects, both acute and delayed**

no data available

#### **Indication of any immediate medical attention and special treatment needed**

no data available

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## SECTION 5: Firefighting measures

#### **Extinguishing media**

Use dry chemical, carbon dioxide or alcohol-resistant foam.

#### **Specific Hazards Arising from the Chemical**

no data available

#### **Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

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## SECTION 6: Accidental release measures

#### **Personal precautions, protective equipment and emergency procedures**

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

#### **Environmental precautions**

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

#### **Methods and materials for containment and cleaning up**

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

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## SECTION 7: Handling and storage

## Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

## Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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# SECTION 8: Exposure controls/personal protection

## Control parameters

### Occupational Exposure limit values

no data available

### Biological limit values

no data available

## Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

## Individual protection measures

### Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

### Skin protection

Wear fire/flamm resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

### Thermal hazards

no data available

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# SECTION 9: Physical and chemical properties

## Information on basic physicochemical properties

Physical state	Solid
Colour	White to Off-White
Odour	no data available
Melting point/freezing point	212°C
Boiling point or initial boiling point and boiling range	564.1°C at 760mmHg
Flammability	no data available
Lower and upper explosion	no data available

limit/flammability limit

Flash point	295°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	DMSO (Slightly), Methanol (Slightly), Phosphoric Acid (Slightly), Water (Slightl
Partition coefficient n-octanol/water	no data available
Vapour pressure	1.46E-13mmHg at 25°C
Density and/or relative density	no data available
Relative vapour density	no data available
Particle characteristics	no data available

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## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

no data available

### Possibility of hazardous reactions

no data available

### Conditions to avoid

no data available

### Incompatible materials

no data available

### Hazardous decomposition products

no data available

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## SECTION 11: Toxicological information

### Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

### Skin corrosion/irritation

no data available

**Serious eye damage/irritation**

no data available

**Respiratory or skin sensitization**

no data available

**Germ cell mutagenicity**

no data available

**Carcinogenicity**

no data available

**Reproductive toxicity**

no data available

**STOT-single exposure**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

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## SECTION 12: Ecological information

**Toxicity**

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

**Persistence and degradability**

no data available

**Bioaccumulative potential**

no data available

**Mobility in soil**

no data available

**Other adverse effects**

no data available

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## SECTION 13: Disposal considerations

### Disposal methods

#### Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

#### Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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## SECTION 14: Transport information

### UN Number

ADR/RID: no data available

IMDG: no data available

IATA: no data available

### UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

### Transport hazard class(es)

ADR/RID: no data available

IMDG: no data available

IATA: no data available

### Packing group, if applicable

ADR/RID: no data available

IMDG: no data available

IATA: no data available

### Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

### Special precautions for user

no data available

### Transport in bulk according to IMO instruments

no data available

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## SECTION 15: Regulatory information

### Safety, health and environmental regulations specific for the product in question

#### European Inventory of Existing Commercial Chemical Substances (EINECS)

Not Listed.

#### EC Inventory

Not Listed.

#### United States Toxic Substances Control Act (TSCA) Inventory

Not Listed.

#### China Catalog of Hazardous chemicals 2015

Not Listed.

#### New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

#### PICCS

Not Listed.

#### Vietnam National Chemical Inventory

Not Listed.

#### IECSC

Not Listed.

#### Korea Existing Chemicals List (KECL)

Not Listed.

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## SECTION 16: Other information

### Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

### References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: <http://www.echemportal.org/echemportal/index?>



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CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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