# Chemical Safety Data Sheet MSDS / SDS

# (3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)-4,5,6,6a-tetrahydro-3aH-cyclopenta[d]isoxazole-6-carboxylic acid

Revision Date:2023-07-15 Revision Number:1

# SECTION 1: Identification of the substance/mixture and of the company/undertaking

#### **Product identifier**

Product name : (3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)-4,5,6,6a-tetrahydro-3aH-

cyclopenta[d]isoxazole-6-carboxylic acid

CBnumber : CB12582792

CAS : 316173-28-1

EINECS Number : 1312995-182-4

Synonyms: (3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(tert-butoxycarbonylaMinoxycarbonylaMinoxycarbonylaMinoxycarbonylaMinoxycarbonylaMinoxycarbonylaMinoxycarbonylaM

butoxycarbonylaMino)-3-(pentan-3-yl)-4,5,6,6a-tetrahydro-3aH-cyclopenta[d]isoxazole-6-carboxylic

acid

### 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 : 400-158-6606

# **SECTION 2: Hazards identification**

### Classification of the substance or mixture

no data available

# Label elements

### Pictogram(s)

Signal word no data available

#### Hazard statement(s)

no data available

### Precautionary statement(s)

#### Prevention

no data available

### Response

no data available

#### Storage

no data available

#### Disposal

no data available

#### Other hazards

no data available

# SECTION 3: Composition/information on ingredients

#### **Substance**

Product name : (3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)-4,5,6,6a-tetrahydro-3aH-

cyclopenta[d]isoxazole-6-carboxylic acid

Synonyms: (3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)-3-(pentan-3-yl)...,(3aR,4R,6S,6aS)-4-(tert-butoxycarbonylaMino)

butoxycarbonylaMino)-3-(pentan-3-yl)-4,5,6,6a-tetrahydro-3aH-cyclopenta[d]isoxazole-6-carboxylic

acid

CAS : 316173-28-1 EC number : 1312995-182-4 MF : C21H39N3O5

MW : 413.56

# 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

# 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.

# 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.

# 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.

# 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 riskelimination 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/flame 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

# SECTION 9: Physical and chemical properties

# Information on basic physicochemical properties

Physical state	no data available
Colour	no data available
Odour	no data available
Melting point/freezing point	no data available
Boiling point or initial boiling point and	no data available
boiling range	
Flammability	no data available
Lower and upper explosion	no data available
limit/flammability limit	
Flash point	no data available
Auto-ignition temperature	no data available
Decomposition temperature	no data available
рН	no data available
Kinematic viscosity	no data available
Solubility	no data available
Partition coefficient n-octanol/water	no data available
Vapour pressure	no data available
Density and/or relative density	no data available
Relative vapour density	no data available
Particle characteristics	no data available

# 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

# **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

# **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

# 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.

# **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

# 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.

# 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?pageID=0&request\_locale=en

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

ChemlDplus, 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/

#### Disclaimer:

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