



according to Regulation (EC) No 1907/2006

## Boc, Pbf-amidino-O1Pen-OH

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

## 1.1. Product identifier

Boc.Pbf-amidino-O1Pen-OH

### Further trade names

Boc, Pbf-amidino-AEA, 5-[N-t-Butyloxycarbonyl-N'-

(2,2,4,6,7-pentamethyldihydrobenzofuran-5-sulfonyl)]amidino-3-oxapentanoic acid, [2-

(N-Boc-N'-Pbf-amidino)ethoxy]acetic acid

CAS No: 1263049-05-3

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

#### Use of the substance/mixture

Laboratory chemical. Manufacture of the substance.

### Uses advised against

Do not use for private purposes (household).

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

Company name: Iris Biotech GmbH

Street: Adalbert-Zoellner-Straße 1
Place: D-95615 Marktredwitz, Germany

Post-office box: 568

D-95605 Marktredwitz, Germany

Telephone: +49 9231 97121 0 Telefax: +49 9231 97121 99

e-mail: info@iris-biotech.de

Contact person: Compliance Department Telephone: +49 9231 97121 0

e-mail: sds@iris-biotech.de Internet: www.iris-biotech.de

Responsible Department: Only available during office hours.

**1.4. Emergency telephone** +49 (0)89 19240 (POISON CENTER Munich: 24 h)

number:

## **Further Information**

This product does not meet the criteria for classification into a hazardous class according to Regulation (EC) No 1272/2008 on the classification, labeling and packaging of substances and mixtures. A safety data sheet is provided which does not fully comply with Article 31 and Annex II of REACH.

Voluntary safety information following the Safety Data Sheet format according to Regulation (EC) No. 1907/2006 (REACH)

### **SECTION 2: Hazards identification**

### 2.1. Classification of the substance or mixture

#### Regulation (EC) No. 1272/2008

This substance is not classified as hazardous in accordance with Regulation (EC) No. 1272/2008.

## 2.2. Label elements

### Regulation (EC) No. 1272/2008

## **Precautionary statements**

P202 Do not handle until all safety precautions have been read and understood.

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

P262 Do not get in eyes, on skin, or on clothing.

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

protection.



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#### Additional advice on labelling

Warning - substance not yet tested completely.

#### 2.3. Other hazards

No information available.

## **SECTION 3: Composition/information on ingredients**

#### 3.1. Substances

#### **Chemical characterization**

Boc, Pbf-amidino-AEA, 5-[N-t-Butyloxycarbonyl-N'-

(2,2,4,6,7-pentamethyldihydrobenzofuran-5-sulfonyl)]amidino-3-oxapentanoic acid, [2-

(N-Boc-N'-Pbf-amidino)ethoxy]acetic acid

Sum formula: C23H35N3O8S Molecular weight: 513.61 g/mol

### **SECTION 4: First aid measures**

#### 4.1. Description of first aid measures

### **General information**

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

## After inhalation

Provide fresh air. Remove casualty to fresh air and keep warm and at rest. In case of irregular breathing or respiratory arrest provide artificial respiration.

In all cases of doubt, or when symptoms persist, seek medical advice.

## After contact with skin

Wash with plenty of water. Take off contaminated clothing and wash it before reuse. After contact with skin, wash immediately with plenty of water and soap.

In all cases of doubt, or when symptoms persist, seek medical advice.

### After contact with eyes

Rinse immediately carefully and thoroughly with eye-bath or water. If product gets into the eye, keep eyelid open and rinse immediately with large quantities of water, for at least 5 minutes. Subsequently consult an ophthalmologist.

### After ingestion

Rinse mouth immediately and drink plenty of water. Rinse mouth thoroughly with water. Never give anything by mouth to an unconscious person or a person with cramps.

In all cases of doubt, or when symptoms persist, seek medical advice.

## 4.2. Most important symptoms and effects, both acute and delayed

No information available.

## 4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

# **SECTION 5: Firefighting measures**

## 5.1. Extinguishing media

#### Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings. Water spray. alcohol resistant foam. Dry extinguishing powder. Carbon dioxide (CO2). Sand.





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### Unsuitable extinguishing media

High power water jet.

#### 5.2. Special hazards arising from the substance or mixture

Non-flammable. Thermal decomposition can lead to the escape of irritating gases and vapours. In case of fire may be liberated: Carbon dioxide (CO2). Carbon monoxide (CO). Nitrogen oxides (NOx).

### 5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.

#### Additional information

Usual measures for fire prevention.

#### **SECTION 6: Accidental release measures**

#### 6.1. Personal precautions, protective equipment and emergency procedures

#### General advice

Provide adequate ventilation. Avoid breathing dust/fume/gas/mist/vapours/spray.

Avoid contact with skin, eyes and clothes.

Wear personal protection equipment.

In case of fire: Evacuate area.

#### 6.2. Environmental precautions

Do not allow to enter into soil/subsoil.

Do not allow to enter into surface water or drains.

#### 6.3. Methods and material for containment and cleaning up

### Other information

Take up mechanically. Treat the recovered material as prescribed in the section on waste disposal. Take up mechanically, placing in appropriate containers for disposal. Avoid dust formation.

Clear contaminated areas thoroughly.

### 6.4. Reference to other sections

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13

# **SECTION 7: Handling and storage**

## 7.1. Precautions for safe handling

### Advice on safe handling

Provide adequate ventilation.

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

Avoid contact with skin, eyes and clothes.

# Advice on protection against fire and explosion

Usual measures for fire prevention.

# Advice on general occupational hygiene

Take off contaminated clothing. Wash hands before breaks and after work. When using do not eat, drink, smoke, sniff. Avoid contact with skin, eyes and clothes. Provide adequate ventilation.

### 7.2. Conditions for safe storage, including any incompatibilities

## Requirements for storage rooms and vessels

Keep container tightly closed in a cool, well-ventilated place.

Handle and store contents under inert gas. Protect from moisture.

storage temperature: +2°C - +8°C

#### Hints on joint storage

No special measures are necessary.

#### 7.3. Specific end use(s)





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Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

### **SECTION 8: Exposure controls/personal protection**

#### 8.1. Control parameters

#### Additional advice on limit values

To date, no national critical limit values exist.

### 8.2. Exposure controls

## Appropriate engineering controls

The receiver of our product is singularly responsible for adhering to existing laws and regulations.

#### Individual protection measures, such as personal protective equipment

#### Eye/face protection

Wear eye/face protection.

#### Hand protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. Wear suitable gloves.

### Skin protection

Use of protective clothing.

## Respiratory protection

In case of inadequate ventilation wear respiratory protection. If technical exhaust or ventilation measures are not possible or insufficient, respiratory protection must be worn.

## **Environmental exposure controls**

Discharge into the environment must be avoided.

### **SECTION 9: Physical and chemical properties**

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

Physical state: Powder
Colour: white/ whitish
Odour: No data available

## Changes in the physical state

Melting point/freezing point:

Boiling point or initial boiling point and

not determined

boiling range:

Sublimation point: not determined

Softening point: not determined

Flash point: No data available

# Flammability

Solid/liquid: not determined
Gas: not applicable

## **Explosive properties**

The product is not: Explosive.

Lower explosion limits:

Upper explosion limits:

not determined

not determined

Auto-ignition temperature:

not determined





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Self-ignition temperature

Solid: not determined Gas: not applicable
Decomposition temperature: not determined pH-Value: not determined
Water solubility: No data available

Solubility in other solvents

not determined

Partition coefficient n-octanol/water:

Vapour pressure:

Density:

not determined

not determined

not determined

not determined

not determined

not determined

9.2. Other information

Information with regard to physical hazard classes

Sustaining combustion: No data available

Oxidizing properties

No data available

Other safety characteristics

Solvent content:

Solid content:

No data available

not determined

Evaporation rate:

not determined

**Further Information** 

## **SECTION 10: Stability and reactivity**

## 10.1. Reactivity

No data available

### 10.2. Chemical stability

Stable under recommended storage conditions.

# 10.3. Possibility of hazardous reactions

No data available

#### 10.4. Conditions to avoid

Protect from moisture.

Keep away from heat.

## 10.5. Incompatible materials

Oxidizing agents, strong.

### 10.6. Hazardous decomposition products

Thermal decomposition can lead to the escape of irritating gases and vapours.

In case of fire may be liberated: Carbon dioxide (CO2). Carbon monoxide (CO). Nitrogen oxides (NOx).

## **Further information**

In case of fire: See chapter 5.

# **SECTION 11: Toxicological information**

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

#### Toxicocinetics, metabolism and distribution

No data available





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### **Acute toxicity**

Based on available data, the classification criteria are not met.

#### Irritation and corrosivity

Based on available data, the classification criteria are not met.

### Sensitising effects

Based on available data, the classification criteria are not met.

### Carcinogenic/mutagenic/toxic effects for reproduction

Based on available data, the classification criteria are not met.

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

#### STOT-single exposure

Based on available data, the classification criteria are not met.

### STOT-repeated exposure

Based on available data, the classification criteria are not met.

#### **Aspiration hazard**

Based on available data, the classification criteria are not met.

### Specific effects in experiment on an animal

No data available

#### Additional information on tests

The substance is classified as not hazardous according to regulation (EC) No 1272/2008 [CLP].

## **Practical experience**

No data available

### **Further information**

RTECS: No data available

Caution! To the best of our knowledge the toxicological properties of this material have not been thoroughly investigated.

## **SECTION 12: Ecological information**

#### 12.1. Toxicity

No data available

#### 12.2. Persistence and degradability

No data available

# 12.3. Bioaccumulative potential

No data available

# 12.4. Mobility in soil

No data available

## 12.5. Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

# 12.7. Other adverse effects

Warning - substance not yet tested completely.

#### **Further information**

Avoid release to the environment.

### **SECTION 13: Disposal considerations**

#### 13.1. Waste treatment methods

### **Disposal recommendations**

Dispose of waste according to applicable legislation.

Consult the appropriate local waste disposal expert about waste disposal.





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Handle contaminated packages in the same way as the substance itself.

### Contaminated packaging

Wash with plenty of water. Completely emptied packages can be recycled.

## **SECTION 14: Transport information**

Land transport (ADR/RID)

**14.2. UN proper shipping name:** No dangerous good in sense of these transport regulations.

Inland waterways transport (ADN)

**14.2. UN proper shipping name:** No dangerous good in sense of these transport regulations.

Marine transport (IMDG)

**14.2. UN proper shipping name:** No dangerous good in sense of these transport regulations.

Air transport (ICAO-TI/IATA-DGR)

**14.2. UN proper shipping name:** No dangerous good in sense of these transport regulations.

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

#### 14.6. Special precautions for user

No information available.

### 14.7. Maritime transport in bulk according to IMO instruments

not applicable

### **SECTION 15: Regulatory information**

### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

#### **EU** regulatory information

Information according to 2012/18/EU Not subject to 2012/18/EU (SEVESO III)

(SEVESO III):

#### **Additional information**

Safety Data Sheet according to Regulation (EC) No. 1907/2006 (REACH)

# **National regulatory information**

Water hazard class (D): 3 - highly hazardous to water

## 15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

### **SECTION 16: Other information**

## Abbreviations and acronyms

ADR: Accord européen sur le transport des marchandises dangereuses par Route

(European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service

LC50: Lethal concentration, 50%

LD50: Lethal dose, 50%

CLP: Classification, labelling and Packaging

REACH: Registration, Evaluation and Authorization of Chemicals

GHS: Globally Harmonised System of Classification, Labelling and Packaging of Chemicals





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**UN: United Nations** 

DNEL: Derived No Effect Level
DMEL: Derived Minimal Effect Level
PNEC: Predicted No Effect Concentration

ATE: Acute toxicity estimate LL50: Lethal loading, 50% EL50: Effect loading, 50%

EC50: Effective Concentration 50%

ErC50: Effective Concentration 50%, growth rate NOEC: No Observed Effect Concentration

BCF: Bio-concentration factor

PBT: persistent, bioaccumulative, toxic vPvB: very persistent, very bioaccumulative

RID: Regulations concerning the international carriage of dangerous goods by rail

ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways (Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures)

EmS: Emergency Schedules MFAG: Medical First Aid Guide

ICAO: International Civil Aviation Organization

MARPOL: International Convention for the Prevention of Marine Pollution from Ships

IBC: Intermediate Bulk Container SVHC: Substance of Very High Concern

For abbreviations and acronyms, see table at http://abbrev.esdscom.eu

#### **Further Information**

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights. The receiver of our product is singularly responsible for adhering to existing laws and regulations.