

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Boc-L-Sec(Mob)-OH

Revision date: 13.04.2023

Product code: BAA3760

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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**

Boc-L-Sec(Mob)-OH

Further trade names

N-alpha-t-Butyloxycarbonyl-Se-(4-methoxybenzyl)-L-selenocysteine

Boc-Sec(PMB)-OH, Boc-Sec(pMeOBzl)-OH

(R)-2-(t-butoxycarbonylamino)-3-(4-methoxybenzylselanyl)propanoic acid

(R)-2-((tert-butoxycarbonyl)amino)-3-((4-methoxybenzyl)selanyl)propanoic acid

CAS No: 959415-39-5

1.2. Relevant identified uses of the substance or mixture and uses advised against**Use of the substance/mixture**

Laboratory chemical.

Scientific research and development

Uses advised against

Do not use for private purposes (household).

Restrictions on use: Pharmaceutical substance

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 number: +49 (0)89 19240 (POISON CENTER Munich: 24 h)**SECTION 2: Hazards identification****2.1. Classification of the substance or mixture****Regulation (EC) No 1272/2008**

Acute Tox. 3; H331

Acute Tox. 3; H301

STOT RE 2; H373

Aquatic Acute 1; H400

Aquatic Chronic 1; H410

Full text of hazard statements: see SECTION 16.

2.2. Label elements**Regulation (EC) No 1272/2008****Signal word:** Danger**Pictograms:**

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Hazard statements

- H301+H331 Toxic if swallowed or if inhaled.
 H373 May cause damage to organs through prolonged or repeated exposure.
 H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

- P260 Do not breathe dust/fume/gas/mist/vapours/spray.
 P264 Wash hands thoroughly after handling.
 P270 Do not eat, drink or smoke when using this product.
 P273 Avoid release to the environment.
 P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.
 P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 P311 Call a POISON CENTER/doctor.
 P314 Get medical advice/attention if you feel unwell.
 P391 Collect spillage.
 P403+P233 Store in a well-ventilated place. Keep container tightly closed.
 P501 Dispose of contents/container to an approved disposal site.

Additional advice on labelling

Warning - substance not yet tested completely.

Labelling of packages where the contents do not exceed 125 ml
Signal word: Danger

Pictograms:

Hazard statements

H301+H331

Precautionary statements

P264-P270-P301+P310-P304+P340-P311-P403+P233-P501

2.3. Other hazards

No information available.

SECTION 3: Composition/information on ingredients
3.1. Substances
Chemical characterization

(R)-2-((tert-butoxycarbonyl)amino)-3-((4-methoxybenzyl)selenanyl)propanoic acid

 Sum formula: C₁₆H₂₃NO₅Se

Molecular weight: 388,33 g/mol

Hazardous components

CAS No	Chemical name	Quantity
	EC No	
	Index No	
	REACH No	
	Classification (Regulation (EC) No 1272/2008)	
959415-39-5	N-alpha-t-Butyloxycarbonyl-Se-(4-methoxybenzyl)-L-selenocysteine	<= 100 %
	Acute Tox. 3, Acute Tox. 3, STOT RE 2, Aquatic Acute 1, Aquatic Chronic 1; H331 H301 H373 H400 H410	

Full text of H and EUH statements: see section 16.

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Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
959415-39-5		N-alpha-t-Butyloxycarbonyl-Se-(4-methoxybenzyl)-L-selenocysteine	<= 100 % %
		inhalation: ATE = 3 mg/l (vapours); inhalation: ATE = 0,5 mg/l (dusts or mists); oral: ATE = 100 mg/kg	

SECTION 4: First aid measures**4.1. Description of first aid measures****General information**

First aider: Pay attention to self-protection! Remove affected person from the danger area and lay down. 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. If breathing is irregular or stopped, administer artificial respiration. No mouth-to-mouth or mouth-to-nose resuscitation. Use Ambu bag or ventilator. Call a physician immediately. 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. Immediately remove any contaminated clothing, shoes or stockings. Medical treatment necessary. 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

After eye contact: Rinse immediately carefully and thoroughly with eye-bath or water. Consult an ophthalmologist.

After ingestion

Induce vomiting when the affected person is not unconscious. Call a physician immediately. 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.

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 (NO_x).

Selenium/Selenium oxides.

5.3. Advice for firefighters

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

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Additional information

Suppress gases/vapours/mists with water spray jet. Collect contaminated fire extinguishing water separately.
Do not allow entering drains or surface water. 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.

For non-emergency personnel

Take up carefully when dry.

For emergency responders

Take up mechanically, placing in appropriate containers for disposal. Take up dust-free and set down dust-free.

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**For containment**

Avoid dust formation.

For cleaning up

Take up mechanically.

Other information

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

Treat the recovered material as prescribed in the section on waste disposal.

SECTION 7: Handling and storage**7.1. Precautions for safe handling****Advice on safe handling**

If handled uncovered, arrangements with local exhaust ventilation have to be used. Avoid dust formation. Do not breathe dust. 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

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme.
Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat or

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

7.2. Conditions for safe storage, including any incompatibilities**Requirements for storage rooms and vessels**

Keep container tightly closed. Keep locked up. Store in a place accessible by authorized persons only. Provide adequate ventilation as well as local exhaust at critical locations. 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)

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**

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe dust. 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. Tightly fitting safety goggles. Face shield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

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.

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Skin protection

Wear suitable 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.

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Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Thermal hazards

No data available

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:	solid	
Colour:	white/ whitish	
Odour:	No data available	
Odour threshold:	not determined	
Melting point/freezing point:		not determined
Boiling point or initial boiling point and boiling range:		not determined
Flammability:		not determined
Lower explosion limits:		not determined
Upper explosion limits:		not determined
Flash point:		No data available
Auto-ignition temperature:		not determined
Decomposition temperature:		not determined
pH-Value:		not determined
Viscosity / kinematic:		not applicable
Water solubility:		No data available
Solubility in other solvents		not determined
Dissolution rate:		not determined
Partition coefficient n-octanol/water:		not determined
Dispersion stability:		No data available
Vapour pressure:		not determined
Density:		not determined
Relative density:		not determined
Bulk density:		not determined
Relative vapour density:		not determined
Particle characteristics:		No data available

9.2. Other information
Information with regard to physical hazard classes

Explosive properties	
No data available	
Sustaining combustion:	No data available
Self-ignition temperature	
Solid:	not determined
Gas:	not applicable
Oxidizing properties	
No data available	

Other safety characteristics

Evaporation rate:	not determined
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Solvent content:	No data available
Solid content:	not determined
Sublimation point:	not determined
Softening point:	not determined
Viscosity / dynamic:	not applicable
Flow time:	not applicable

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 (NO_x).

Selenium/Selenium oxides.

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

Toxicokinetics, metabolism and distribution

No data available

Acute toxicity

Toxic if swallowed.

Toxic if inhaled.

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
959415-39-5	N-alpha-t-Butyloxycarbonyl-Se-(4-methoxybenzyl)-L-selenocysteine				
	oral	ATE 100 mg/kg			
	inhalation vapour	ATE 3 mg/l			
	inhalation dust/mist	ATE 0,5 mg/l			

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

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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

May cause damage to organs through prolonged or repeated exposure. (N-alpha-t-Butyloxycarbonyl-Se-(4-methoxybenzyl)-L-selenocysteine)

Aspiration hazard

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

Specific effects in experiment on an animal

No data available

Practical experience

No data available

11.2. Information on other hazards**Endocrine disrupting properties**

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. Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information**12.1. Toxicity**

Very toxic to aquatic life.

Very toxic to aquatic life with long lasting effects.

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

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

12.7. Other adverse effects

Warning - substance not yet tested completely.

Further information

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations**13.1. Waste treatment methods****Disposal recommendations**

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil. Dispose of waste according to applicable legislation. 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

This material and its container must be disposed of as hazardous waste. Handle contaminated packages in the same way as the substance itself.


SECTION 14: Transport information**Land transport (ADR/RID)**

14.1. UN number or ID number:	UN 3283
14.2. UN proper shipping name:	SELENIUM COMPOUND, SOLID, N.O.S. ((R)-2-((tert-butoxycarbonyl)amino)-3-((4-methoxybenzyl)selenyl)propanoic acid)
14.3. Transport hazard class(es):	6.1
14.4. Packing group:	II
Hazard label:	6.1
	
Classification code:	T5
Special Provisions:	274 563
Limited quantity:	500 g
Excepted quantity:	E4
Transport category:	2
Hazard No:	60
Tunnel restriction code:	D/E

Inland waterways transport (ADN)

14.1. UN number or ID number:	UN 3283
14.2. UN proper shipping name:	SELENIUM COMPOUND, SOLID, N.O.S. ((R)-2-((tert-butoxycarbonyl)amino)-3-((4-methoxybenzyl)selenyl)propanoic acid)
14.3. Transport hazard class(es):	6.1
14.4. Packing group:	II
Hazard label:	6.1
	
Classification code:	T5
Special Provisions:	274 563 802
Limited quantity:	500 g
Excepted quantity:	E4

Marine transport (IMDG)

14.1. UN number or ID number:	UN 3283
14.2. UN proper shipping name:	SELENIUM COMPOUND, SOLID, N.O.S. ((R)-2-((tert-butoxycarbonyl)amino)-3-((4-methoxybenzyl)selenyl)propanoic acid)
14.3. Transport hazard class(es):	6.1
14.4. Packing group:	II
Hazard label:	6.1
	
Special Provisions:	274

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Limited quantity: 500 g
 Excepted quantity: E4
 EmS: F-A, S-A

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number: UN 3283
14.2. UN proper shipping name: SELENIUM COMPOUND, SOLID, N.O.S. ((R)-2-((tert-butoxycarbonyl)amino)-3-((4-methoxybenzyl)selanyl)propanoic acid)
14.3. Transport hazard class(es): 6.1
14.4. Packing group: II
 Hazard label: 6.1



Special Provisions: A3 A5
 Limited quantity Passenger: 1 kg
 Passenger LQ: Y644
 Excepted quantity: E4
 IATA-packing instructions - Passenger: 669
 IATA-max. quantity - Passenger: 25 kg
 IATA-packing instructions - Cargo: 676
 IATA-max. quantity - Cargo: 100 kg

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: Yes



Danger releasing substance: (R)-2-((tert-butoxycarbonyl)amino)-3-((4-methoxybenzyl)selanyl)propanoic acid

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 (SEVESO III): H2 ACUTE TOXIC
 Additional information: E1

National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.
 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

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Changes

This data sheet contains changes from the previous version in section(s): 1,2.

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%

Relevant H and EUH statements (number and full text)

H301	Toxic if swallowed.
H301+H331	Toxic if swallowed or if inhaled.
H331	Toxic if inhaled.
H373	May cause damage to organs through prolonged or repeated exposure.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

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.