

Safety Data Sheet

according to UK REACH Regulation

Boc-2-amino-4,4,4-trifluoro-butyric acid (S)

Revision date: 31.03.2020

Product code: BAA2140

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

Boc-2-amino-4,4,4-trifluoro-butyric acid (S)

Further trade names

(S)-2-t-Butyloxycarbonylamino-4,4,4-trifluoro-butyric acid

(S)-Boc-2-amino-4,4,4-trifluoro-butyric acid

Substance name: Boc-2-amino-4,4,4-trifluoro-butyric acid (S)

CAS No: 181128-25-6

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 number: +49 (0)89 19240 (POISON CENTER Munich: 24 h)**Further information:****Further Information**

Emergency telephone: 24 h (POISON CENTER Munich)

SECTION 2: Hazards identification**2.1. Classification of the substance or mixture****GB CLP Regulation**

Hazard categories:

Skin corrosion/irritation: Skin Irrit. 2

Serious eye damage/eye irritation: Eye Irrit. 2

Specific target organ toxicity - single exposure: STOT SE 3

Hazard Statements:

Causes skin irritation.

Causes serious eye irritation.

May cause respiratory irritation.

2.2. Label elements**GB CLP Regulation**

Signal word: Warning

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Pictograms:

Hazard statements

H315 Causes skin irritation.
 H319 Causes serious eye irritation.
 H335 May cause respiratory irritation.

Precautionary statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
 P264 Wash hands thoroughly after handling.
 P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
 P302+P352 IF ON SKIN: Wash with plenty of Water.
 P332+P313 If skin irritation occurs: Get medical advice/attention.
 P362+P364 Take off contaminated clothing and wash it before reuse.
 P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 P312 Call a POISON CENTER/doctor if you feel unwell.
 P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 P337+P313 If eye irritation persists: Get medical advice/attention.
 P403+P233 Store in a well-ventilated place. Keep container tightly closed.
 P405 Store locked up.
 P501 Dispose of contents/container to an approved disposal site.

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

N-alpha-t-Butyloxycarbonyl-3-iodo-L-phenylalanine

 Sum formula: C₉H₁₄F₃NO₄

Molecular weight: 257,21 g/mol

Hazardous components

CAS No	Chemical name	Index No	REACH No	Quantity
	EC No			
	GHS Classification			
181128-25-6	Boc-2-amino-4,4,4-trifluoro-butyric acid (S)			<= 100 %
	Skin Irrit. 2, Eye Irrit. 2, STOT SE 3; H315 H319 H335			

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

SECTION 4: First aid measures
4.1. Description of first aid measures

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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. Medical treatment necessary. 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

Take off immediately all contaminated clothing and wash it before reuse. If skin irritation occurs: Get medical advice/attention. 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

In case of contact with eyes, rinse immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart. Subsequently consult an ophthalmologist.

After ingestion

Rinse mouth immediately and drink 1 glass 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.

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). Fluorhydric acid.

5.3. Advice for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing. Full protection suit.

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 measures**

Avoid dust formation. Do not breathe dust. Avoid contact with skin, eyes and clothes. Use personal protection equipment. Provide adequate ventilation. Avoid breathing dust/fume/gas/mist/vapours/spray. Wear personal protection equipment. In case of fire: Evacuate area.

6.2. Environmental precautions

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

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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

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, 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. Keep locked up. Store in a place accessible by authorized persons only.

Provide adequate ventilation as well as local exhaustion 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

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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**

Suitable eye protection: goggles.

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:	solid
Colour:	white/ whitish
Odour:	No data available

Changes in the physical state

Melting point/freezing point:	not determined
Boiling point or initial boiling point and boiling range:	not determined
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:	not determined
Upper explosion limits:	not determined
Auto-ignition temperature:	not determined

Self-ignition temperature

Solid:	not determined
Gas:	not applicable

Decomposition temperature:	not determined
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Oxidizing properties

No data available

pH-Value:	not determined
Water solubility:	No data available

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Solubility in other solvents

Soluble in: Dimethylformamide (DMF): 1 mmol in 2 ml DMF.

Partition coefficient n-octanol/water:	not determined
Vapour pressure:	not determined
Density:	not determined
Relative vapour density:	not determined

9.2. Other information**Information with regard to physical hazard classes**

Sustaining combustion: No data available

Other safety characteristics

Solvent content:	No data available
Solid content:	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 avoidProtect from moisture.
Keep away from heat.**10.5. Incompatible materials**

Oxidizing agents, strong.

10.6. Hazardous decomposition productsThermal 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).
Fluorhydric acid..**Further information**

In case of fire: See chapter 5.

SECTION 11: Toxicological information**11.1. Information on hazard classes as defined in GB CLP Regulation****Toxicokinetics, metabolism and distribution**

No data available

Acute toxicity

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

Irritation and corrosivityCauses skin irritation.
Causes serious eye irritation.**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

May cause respiratory irritation. (Boc-2-amino-4,4,4-trifluoro-butyric acid (S))

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

Classification according to Regulation (EC) No 1272/2008 [CLP]: health hazard properties

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.

Handle in accordance with good industrial hygiene and safety practice.

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

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

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.

Consult the appropriate local waste disposal expert about waste disposal.

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

Contaminated packaging

Non-contaminated packages may be recycled. Handle contaminated packages in the same way as the substance itself.

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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 (SEVESO III): Not subject to 2012/18/EU (SEVESO III)

Additional information

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

National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC).

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

UN: United Nations

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CAS: Chemical Abstracts Service
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
IATA: International Air Transport Association
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>

Relevant H and EUH statements (number and full text)

H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

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.