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



Boc-L-Isoleucine hemihydrate PEPTIPURE® ≥98 %, for biochemistry

article number: **6923** date of compilation: 2021-08-11

Version: **1.0 en**

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

1.1 Product identifier

Identification of the substance **Boc-L-Isoleucine hemihydrate** PEPTIPURE® ≥98

%, for biochemistry

Article number 6923

Registration number (REACH)

It is not required to list the identified uses be-

cause the substance is not subject to registration

according to REACH (< 1 t/a).

EC number 236-074-8 CAS number 13139-16-7

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

Relevant identified uses: Laboratory chemical

Laboratory and analytical use

Uses advised against: Do not use for products which come into contact

with foodstuffs. Do not use for private purposes

(household).

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co KG Schoemperlenstr. 3-5 D-76185 Karlsruhe Germany

Telephone:+49 (0) 721 - 56 06 0 **Telefax:** +49 (0) 721 - 56 06 149 **e-mail:** sicherheit@carlroth.de **Website:** www.carlroth.de

Competent person responsible for the safety data :Department Health, Safety and Environment

sheet:

e-mail (competent person): sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

2.2 Label elements

United Kingdom (en) Page 1 / 11

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



Boc-L-Isoleucine hemihydrate PEPTIPURE® ≥98 %, for biochemistry

article number: 6923

Labelling according to Regulation (EC) No 1272/2008 (CLP)

not required

2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance Boc-L-Isoleucine hemihydrate

Molecular formula $C_{11}H_{21}NO_4\cdot ^12H_2O$

Molar mass 240,3 ⁹/_{mol}
CAS No 13139-16-7
EC No 236-074-8

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air.

Following skin contact

Rinse skin with water/shower.

Following eye contact

Rinse cautiously with water for several minutes.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Symptoms and effects are not known to date.

4.3 Indication of any immediate medical attention and special treatment needed

none

United Kingdom (en) Page 2 / 11

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



Boc-L-Isoleucine hemihydrate PEPTIPURE® ≥98 %, for biochemistry

article number: 6923

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings water, foam, dry extinguishing powder, ABC-powder

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

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

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Control of dust.

6.2 Environmental precautions

Keep away from drains, surface and ground water.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically.

Other information relating to spills and releases

Place in appropriate containers for disposal.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

United Kingdom (en) Page 3 / 11

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



Boc-L-Isoleucine hemihydrate PEPTIPURE® ≥98 %, for biochemistry

article number: 6923

SECTION 7: Handling and storage

7.1 Precautions for safe handling

No special measures are necessary.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place. Keep in a cool place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ventilation requirements

Use local and general ventilation.

Specific designs for storage rooms or vessels

Recommended storage temperature: 2 - 8 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Coun try	Name of agent	CAS No	Identifi- er	TWA [mg/ m³]	STEL [mg/ m³]	Ceil- ing-C [mg/ m³]	Nota- tion	Source
GB	dust		WEL	10			i	EH40/2005
GB	dust		WEL	4			r	EH40/2005

Notation

Ceiling-C Ceiling value is a limit value above which exposure should not occur Inhalable fraction

r Respirable fraction

STEL Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-

minute period (unless otherwise specified)

TWA Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8

hours time-weighted average (unless otherwise specified)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

United Kingdom (en) Page 4 / 11

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



Boc-L-Isoleucine hemihydrate PEPTIPURE® ≥98 %, for biochemistry

article number: 6923

Skin protection



hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374.

• type of material

NBR (Nitrile rubber)

material thickness

>0,11 mm

breakthrough times of the glove material

>480 minutes (permeation: level 6)

other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection





Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P1 (filters at least 80 % of airborne particles, colour code: White).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state solid
Form powder

Colour white - whitish
Odour odourless
Melting point/freezing point 50 – 60 °C

Boiling point or initial boiling point and boiling no

range

not determined

Flammability this material is combustible, but will not ignite

readily

Lower and upper explosion limit not determined
Flash point not applicable
Auto-ignition temperature not determined
Decomposition temperature not relevant
pH (value) not applicable

United Kingdom (en) Page 5 / 11

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



Boc-L-Isoleucine hemihydrate PEPTIPURE® ≥98 %, for biochemistry

article number: 6923

Kinematic viscosity not relevant

Solubility(ies)

Water solubility not determined

Partition coefficient

Partition coefficient n-octanol/water (log value): this information is not available

Vapour pressure not determined

Density not determined

Relative vapour density information on this property is not available

Particle characteristics No data available.

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard hazard classes acc. to GHS

classes: (physical hazards): not relevant

Other safety characteristics: There is no additional information.

SECTION 10: Stability and reactivity

10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser

10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

United Kingdom (en) Page 6 / 11

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

ROTH

Boc-L-Isoleucine hemihydrate PEPTIPURE® ≥98 %, for biochemistry

article number: 6923

SECTION 11: Toxicological information

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

Classification according to GHS (1272/2008/EC, CLP)

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

Acute toxicity

Shall not be classified as acutely toxic.

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

If swallowed

Data are not available.

• If in eyes

Data are not available.

If inhaled

Data are not available.

• If on skin

Data are not available.

Other information

Health effects are not known.

11.2 Endocrine disrupting properties

Not listed.

United Kingdom (en) Page 7 / 11

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



Boc-L-Isoleucine hemihydrate PEPTIPURE® ≥98 %, for biochemistry

article number: 6923

11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Biodegradation

Data are not available.

12.2 Process of degradability

Theoretical Oxygen Demand with nitrification: 2,031 ^{mg}/_{mg} Theoretical Oxygen Demand: 1,798 ^{mg}/_{mg} Theoretical Carbon Dioxide: 2,014 ^{mg}/_{mg}

12.3 Bioaccumulative potential

Data are not available.

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Not listed.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



Consult the appropriate local waste disposal expert about waste disposal.

Sewage disposal-relevant information

Do not empty into drains.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process. Waste catalogue ordinance (Germany).

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions.

United Kingdom (en) Page 8 / 11

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



Boc-L-Isoleucine hemihydrate PEPTIPURE® ≥98 %, for biochemistry

article number: 6923

SECTION 14: Transport information

14.1 UN number or ID number not subject to transport regulations

14.2 UN proper shipping name not assigned

14.3 Transport hazard class(es) none

14.4 Packing group not assigned

14.5 Environmental hazards non-environmentally hazardous acc. to the dan-

gerous goods regulations

14.6 Special precautions for user

There is no additional information.

14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

14.8 Information for each of the UN Model Regulations

Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information

Not subject to ADR, RID and ADN.

International Maritime Dangerous Goods Code (IMDG) - Additional information

Not subject to IMDG.

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Not subject to ICAO-IATA.

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture Relevant provisions of the European Union (EU)

Restrictions according to REACH, Annex XVII

not listed

List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list

Not listed.

Seveso Directive

2012/18/EU (Seveso III)				
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements	Notes	
	not assigned			

Deco-Paint Directive

VOC content	0 %
-------------	-----

Industrial Emissions Directive (IED)

VOC content	0 %
-------------	-----

United Kingdom (en) Page 9 / 11

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

Boc-L-Isoleucine hemihydrate PEPTIPURE® ≥98 %, for biochemistry

article number: 6923

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

Regulation on the marketing and use of explosives precursors

not listed

Regulation on drug precursors

not listed

Regulation on substances that deplete the ozone layer (ODS)

not listed

Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

Regulation on persistent organic pollutants (POP)

not listed

National inventories

Country	Inventory	Status
CA	NDSL	substance is listed
EU	ECSI	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed

Legend

ECSI EC Substance Inventory (EINECS, ELINCS, NLP) Non-domestic Substances List (NDSL) NDSL Taiwan Chemical Substance Inventory Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de naviga- tion intérieures (European Agreement concerning the International Carriage of Dangerous Goods by In- land Waterways)
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	Ceiling value
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures

United Kingdom (en) Page 10 / 11

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



Boc-L-Isoleucine hemihydrate PEPTIPURE® ≥98 %, for biochemistry

article number: 6923

Abbr.	Descriptions of used abbreviations
DGR	Dangerous Goods Regulations (see IATA/DGR)
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
EH40/2005	EH40/2005 Workplace exposure limits (http://www.nationalarchives.gov.uk/doc/open-government-li- cence/)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regula- tions concerning the International carriage of Dangerous goods by Rail)
STEL	Short-term exposure limit
SVHC	Substance of Very High Concern
TWA	Time-weighted average
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative
WEL	Workplace exposure limit

Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures. Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.

United Kingdom (en) Page 11 / 11