

SAFETY DATA SHEET

Version 8.13
Revision Date 04/29/2025
Print Date 04/30/2025

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : PyBOP Novabiochem®

Product Number : 8.51009
Catalogue No. : 851009
Brand : Millipore
CAS-No. : 128625-52-5

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

Identified uses : Peptide synthesis, Chemical for synthesis
Uses advised against :
The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute toxicity (Oral) : Category 4

Skin sensitization : Category 1

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Short-term (acute) aquatic hazard : Category 1

Long-term (chronic) aquatic hazard : Category 1

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal Word : Warning

Hazard Statements : H302 Harmful if swallowed.
H317 May cause an allergic skin reaction.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary Statements : **Prevention:**
P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P272 Contaminated work clothing must not be allowed out of the workplace.
P273 Avoid release to the environment.
P280 Wear protective gloves.
Response:
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P363 Wash contaminated clothing before reuse.
P391 Collect spillage.
Disposal:
P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**Millipore
Sigma**

Components

| Chemical name | CAS No./Unique ID | Concentration (% w/w) | Trade secret |
|---|-------------------|-----------------------|--------------|
| benzotriazol-1-yloxytripyrrolidinophosphonium hexafluorophosphate | 128625-52-5* | >= 90 - <= 100 | - |

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

| | |
|---|--|
| General advice | : Show this material safety data sheet to the doctor in attendance. |
| If inhaled | : After inhalation: fresh air. |
| In case of skin contact | : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician. |
| In case of eye contact | : After eye contact: rinse out with plenty of water. Remove contact lenses. |
| If swallowed | : After swallowing: immediately make victim drink water (two glasses at most). Consult a physician. |
| Most important symptoms and effects, both acute and delayed | : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11 |
| Protection of first-aiders | : For personal protection see section 8. |
| Notes to physician | : No data available |

SECTION 5. FIRE-FIGHTING MEASURES

| | |
|---------------------------------------|--|
| Suitable extinguishing media | : Water Foam Carbon dioxide (CO ₂) Dry powder |
| Unsuitable extinguishing media | : For this substance/mixture no limitations of extinguishing agents are given. |
| Specific hazards during fire fighting | : Combustible. |

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Fire may cause evolution of:

nitrogen oxides
Hydrogen fluoride
Oxides of phosphorus

Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products : Carbon oxides

Nitrogen oxides (NO_x)

Oxides of phosphorus

Hydrogen fluoride

Specific extinguishing methods : No data available

Further information : Suppress (knock down) gases/vapors/mists with a water spray jet.
Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:
Avoid inhalation of dusts.
Avoid substance contact.
Ensure adequate ventilation.
Evacuate the danger area, observe emergency procedures, consult an expert.
Advice for emergency responders:
For personal protection see section 8.

Environmental : Do not let product enter drains.

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precautions

Methods and materials for containment and cleaning up : Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10).
Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Further information on storage conditions : Tightly closed.
Dry.

Storage class : 13, Non Combustible Solids

Recommended storage temperature : Recommended storage temperature see product label.

Further information on storage stability : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type P2

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

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Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Full contact
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Splash contact
Manufacturer : KCL 741 Dermatril® L

Remarks : This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : powder

Color : white, to, off-white

Odor : No data available

Odor Threshold : No data available

pH : No data available

Melting point : < 320 °F / < 160 °C
Decomposition: yes
Method: OECD Test Guideline 102
GLP: yes
(decomposition)

| | |
|---|---|
| Boiling point/boiling range | : No data available |
| Flash point | : No data available |
| Evaporation rate | : No data available |
| Flammability (solid, gas) | : The product is not flammable. Method: Test N.1: Test method for readily combustible solids GLP: yes |
| Burning rate | : No data available |
| Upper explosion limit / Upper flammability limit | : No data available |
| Lower explosion limit / Lower flammability limit | : No data available |
| Vapor pressure | : < 1 hPa (77 °F / 25 °C) Method: OECD Test Guideline 104 GLP: yes |
| Relative vapor density | : No data available |
| Relative density | : No data available |
| Density | : 1.438 g/cm ³ (68 °F / 20 °C) Method: OECD Test Guideline 109 GLP: yes |
| Solubility(ies) Water solubility | : 0.7182 g/l (68 °F / 20 °C) Method: OECD Test Guideline 105 GLP: yes |
| Partition coefficient: n- octanol/water | : No data available |
| Autoignition temperature | : No data available |
| Decomposition temperature | : No data available |
| Viscosity, dynamic | : No data available |
| Viscosity, kinematic | : No data available |
| Flow time | : No data available |
| Explosive properties | : Method: Explosive properties |

| | |
|--------------------------|--|
| Oxidizing properties | : The substance or mixture is not classified as oxidizing. GLP: yes |
| Molecular weight | : 520.39 g/mol |
| Particle characteristics | |
| Particle size | : No data available |

SECTION 10. STABILITY AND REACTIVITY

| | |
|------------------------------------|---|
| Reactivity | : The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed. |
| Chemical stability | : The product is chemically stable under standard ambient conditions (room temperature) . |
| Possibility of hazardous reactions | : Violent reactions possible with: Oxidizing agents |
| Conditions to avoid | : no information available |
| Incompatible materials | : No data available |
| Hazardous decomposition products | : In the event of fire: see section 5 |

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - > 300 - < 2,000 mg/kg

(OECD Test Guideline 423)

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Skin - EPISKIN Human Skin Model Test

Result: No skin irritation

(OECD Test Guideline 439)

Serious eye damage/eye irritation

Eyes - In vitro study

Result: No eye irritation

(OECD Test Guideline 492)

Respiratory or skin sensitization

In Chemico Skin Sensitisation: Direct Peptide Reactivity Assay (DPRA)

Result: positive
(OECD Test Guideline 442C)
In vitro study
Result: positive
(OECD Test Guideline 442D)

Germ cell mutagenicity

Test Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties 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

Ecotoxicity

Components:

benzotriazol-1-yloxytripyrrolidinophosphonium hexafluorophosphate:

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 0.25 mg/l
Exposure time: 48 h
Test Type: semi-static test

Method: OECD Test Guideline 202
GLP: yes

Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata (green algae)): 2.54 mg/l
Exposure time: 72 h
Test Type: static test
Method: OECD Test Guideline 201
GLP: yes

EC10 (Pseudokirchneriella subcapitata (green algae)): 0.52 mg/l
Exposure time: 72 h
Test Type: static test
Method: OECD Test Guideline 201
GLP: yes

M-Factor (Acute aquatic toxicity) : 1

M-Factor (Chronic aquatic toxicity) : 1

Persistence and degradability

Components:

benzotriazol-1-yloxytripyrrolidinophosphonium hexafluorophosphate:

Biodegradability : aerobic
Inoculum: activated sludge, non-adapted
Concentration: 102 mg/l
Result: Not readily biodegradable.
Biodegradation: 0 %
Exposure time: 28 d
Method: OECD Test Guideline 301F
GLP: yes

Bioaccumulative potential

No data available

Mobility in soil

No data available

Other adverse effects

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other

waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 3077
Proper shipping name : Environmentally hazardous substance, solid, n.o.s.
(benzotriazol-1-yloxytripyrrolidinophosphonium hexafluorophosphate)
Class : 9
Packing group : III
Labels : Class 9 - Miscellaneous dangerous substances and articles
Packing instruction (cargo aircraft) : 956
Packing instruction (passenger aircraft) : 956

IMDG-Code

UN number : UN 3077
Proper shipping name : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
(benzotriazol-1-yloxytripyrrolidinophosphonium hexafluorophosphate)
Class : 9
Packing group : III
Labels : 9
EmS Code : F-A, S-F
Marine pollutant : yes

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National regulation

49 CFR Road

Not regulated as a dangerous good

Poison Inhalation Hazard : No

Special precautions for user

Remarks : EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids. Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN -

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Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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