Safety Data Sheet

According to 29 CFR 1910.1200 (OSHA Hazard Communication Standard, 2024)

Version 2 · Date of preparation 2026-10-07

Section 1. Identification

Product identifier used on the label	PyBOP (product number 31010)
Other means of identification	Product number: 31010 Abbreviation: PyBOP Molecular formula: C18H28F6N6OP2 (molecular weight 520.39)
Recommended use of the chemical and restrictions on use	Recommended use: laboratory chemical; peptide coupling (amide bond-forming) reagent for research and for the manufacture of substances. Restrictions on use: not for use in food, drugs, pesticides or biocidal products.
Name, U.S. address, and U.S. telephone number of the chemical manufacturer, importer, or other responsible party	P3 BioSystems 270 Haven Hill Rd, Shelbyville, KY 40065 Telephone: +1 888-737-5598 Email: info@p3bio.com
Emergency phone number	+1 888-737-5598 (P3 BioSystems office line, business hours)

Section 2. Hazard identification

Classification of the chemical in accordance with paragraph (d)(1) of § 1910.1200, except for classification under paragraph (d)(1)(ii)	• Acute toxicity - oral, category 4 • Skin corrosion/irritation, category 2 • Eye damage/irritation, category 2A • Specific target organ toxicity (single exposure), category 3 • Sensitization - skin, category 1 (including both sub-categories 1A and 1B)

Signal word, hazard statement(s), symbol(s) and precautionary statement(s) in accordance with paragraph (f) of § 1910.1200	**Signal word: Warning** Hazard pictograms: Exclamation Mark Hazard statements: • H302 Harmful if swallowed. • H315 Causes skin irritation. • H319 Causes serious eye irritation. • H335 May cause respiratory irritation. • H317 May cause an allergic skin reaction. Precautionary statements: • P261 Avoid breathing dust. • P264 Wash hands thoroughly after handling. • P270 Do not eat, drink or smoke when using this product. • P271 Use only outdoors or in a well-ventilated area. • P272 Contaminated work clothing must not be allowed out of the workplace. • P280 Wear protective gloves/eye protection/face protection. • P301+P312 If swallowed: Call a poison center or doctor if you feel unwell. • P330 Rinse mouth. • P302+P352 If on skin: Wash with plenty of soap and water. • P304+P340 If inhaled: Remove person to fresh air and keep comfortable for breathing. • P305+P351+P338 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. • P312 Call a poison center or doctor if you feel unwell. • P321 Specific treatment (see Section 4 of this SDS). • P333+P313 If skin irritation or rash occurs: Get medical advice/attention. • P337+P313 If eye irritation persists: Get medical advice/attention. • P362+P364 Take off contaminated clothing and wash it before reuse. • P405 Store locked up. • P501 Dispose of contents/container in accordance with local, state and federal regulations.
Hazards classified under paragraph (d)(1)(ii) of § 1910.1200	In use as a peptide coupling reagent, PyBOP releases 1-hydroxybenzotriazole (HOBt) and tris(pyrrolidin-1-yl)phosphine oxide as by-products. HOBt causes serious eye irritation and is explosive when dry; do not evaporate reaction mixtures or wastes containing it to dryness. No hazard data were found for tris(pyrrolidin-1-yl)phosphine oxide.
Hazards not otherwise classified that have been identified during the classification process	None identified.

Where an ingredient with unknown acute toxicity is used in a mixture at a concentration ≥ 1% and the mixture is not classified based on testing of the mixture as a whole, a statement that X% of the mixture consists of ingredient(s) of unknown acute toxicity	Not applicable: the product is a substance, not a mixture.

Section 3. Composition/information on ingredients

Chemical name	benzotriazol-1-yloxy(tripyrrolidin-1-yl)phosphanium hexafluorophosphate
Common name and synonyms	PyBOP (Benzotriazol-1-yloxy)tripyrrolidinophosphonium hexafluorophosphate Benzotriazol-1-yl-oxytripyrrolidinophosphonium hexafluorophosphate 1H-Benzotriazol-1-yloxytri(1-pyrrolidinyl)phosphonium hexafluorophosphate
CAS number and other unique identifiers	• CAS number: 128625-52-5 • InChIKey: VIAFLMPQBHAMLI-UHFFFAOYSA-N • PubChem CID: 2724699
Impurities and stabilizing additives (constituents) which are themselves classified and which contribute to the classification of the substance	None known. Purity is at least 99.0% (HPLC), per specification; no impurity or additive is known to contribute to the classification.

Section 4. First-aid measures

Description of necessary measures, subdivided according to the different routes of exposure, i.e., inhalation, skin and eye contact, and ingestion	General advice: Show this safety data sheet to the doctor in attendance. Inhalation: Remove the person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Call a poison center or doctor if you feel unwell. Skin contact: Take off contaminated clothing. Wash the skin with plenty of soap and water for at least 15 minutes. If skin irritation or a rash occurs, get medical advice/attention. Wash contaminated clothing before reuse. Eye contact: Rinse cautiously with plenty of water for at least 15 minutes, also under the eyelids. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists, get medical advice/attention. Ingestion: Rinse mouth. Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Call a poison center or doctor if you feel unwell.

Most important symptoms/effects, acute and delayed	Acute: harmful if swallowed; skin irritation (redness, itching); serious eye irritation (redness, pain, watering); irritation of the nose, throat and airways from dust (coughing, sneezing). Delayed: allergic skin reaction. Symptoms of an allergic reaction may include rash, itching and swelling and, in more severe reactions, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing. Once a person is sensitized, very small amounts can provoke a reaction.
Indication of immediate medical attention and special treatment needed, if necessary	Treat symptomatically. Get medical advice if a rash or other sign of an allergic reaction develops; a sensitized person should avoid any further contact with the product.

Section 5. Fire-fighting measures

Suitable (and unsuitable) extinguishing media	Suitable extinguishing media: water spray, carbon dioxide (CO2), dry chemical, alcohol-resistant foam. Unsuitable extinguishing media: no information available.
Specific hazards arising from the chemical (e.g., nature of any hazardous combustion products)	Not classified as flammable. Hazardous combustion products: carbon monoxide, carbon dioxide, nitrogen oxides (NOx), oxides of phosphorus and hydrogen fluoride.
Special protective equipment and precautions for fire-fighters	Wear a self-contained breathing apparatus (pressure-demand, NIOSH-approved or equivalent) and full protective gear. Do not allow run-off from fire fighting to enter drains or watercourses; the product is very toxic to aquatic life.

Section 6. Accidental release measures

Personal precautions, protective equipment, and emergency procedures	Wear the personal protective equipment described in Section 8, including gloves and eye protection. Avoid dust formation and avoid breathing dust. Avoid contact with skin, eyes and clothing. Ensure adequate ventilation. Keep unprotected people away.
Methods and materials for containment and cleaning up	Prevent the product from entering drains, surface water or groundwater. Pick up without creating dust: sweep up and shovel into a suitable, closed, labelled container for disposal. Clean the affected area. Local authorities should be advised if a significant spillage cannot be contained. Dispose of as described in Section 13.

Section 7. Handling and storage

Precautions for safe handling	Handle in a chemical fume hood or with adequate local exhaust ventilation. Avoid dust formation and avoid breathing dust. Avoid contact with skin, eyes and clothing. Wear protective gloves and eye/face protection (Section 8). Contaminated work clothing must not be allowed out of the workplace. Wash hands thoroughly after handling. Do not eat, drink or smoke when using this product. Avoid release to the environment.

Conditions for safe storage, including any incompatibilities	Store refrigerated (2–8 °C) in a tightly closed container in a dry, well-ventilated place, protected from light (per specification). Store locked up. The product is moisture- and light-sensitive. Incompatible materials: strong oxidizing agents, strong acids, strong bases.

Section 8. Exposure controls/personal protection

OSHA permissible exposure limit (PEL), ACGIH Threshold Limit Value (TLV), and any other exposure limit used or recommended by the chemical manufacturer, importer, or employer preparing the safety data sheet, where available	No OSHA PEL or ACGIH TLV has been established.
Appropriate engineering controls	Use a chemical fume hood or local exhaust ventilation to keep airborne dust as low as possible. Eyewash stations and safety showers should be close to the workstation.
Individual protection measures, such as personal protective equipment	Eye/face protection: chemical safety goggles or safety glasses with side shields meeting OSHA's eye and face protection regulations (29 CFR 1910.133); add a face shield where dust or splashes are likely. Skin protection: nitrile rubber gloves (minimum thickness 0.11 mm; reported breakthrough time 480 min), inspected before use and removed without touching the outer surface; dispose of contaminated gloves after use. Wear a laboratory coat or other protective clothing to prevent skin contact. Respiratory protection: not normally required when the product is handled in a fume hood. Where dust cannot be controlled, use a NIOSH-approved particulate respirator (N95/P95 or better) under a respiratory protection program meeting 29 CFR 1910.134. Hygiene: wash hands before breaks and at the end of work. Do not eat, drink or smoke in the work area.

Section 9. Physical and chemical properties

Physical state	Solid (crystalline powder), per specification.
Color	White to off-white, per specification.
Odor (includes odor threshold)	Odor: no information available. Odor threshold: no information available.
Melting point/freezing point	Melting point: 150–160 °C, per specification. Melts with decomposition.
Boiling point (or initial boiling point or boiling range)	No information available.
Flammability	No test data available. Not classified as a flammable solid.
Lower and upper explosion limit/flammability limit	No data available.

Flash point	No information available.
Auto-ignition temperature	No data available.
Decomposition temperature	No data available.
pH	No information available.
Kinematic viscosity	Not applicable (solid).
Solubility	Water: no information available. Soluble in N,N-dimethylformamide (DMF): 0.3 g in 2 mL gives a clear solution (per specification).
Partition coefficient n-octanol/water (log value)	No data available.
Vapor pressure (includes evaporation rate)	Vapor pressure: no data available. Evaporation rate: not applicable (solid).
Density and/or relative density	No data available.
Relative vapor density	Not applicable (solid).
Particle characteristics	No data available.

Section 10. Stability and reactivity

Reactivity	No hazardous reactivity known, based on the information available.
Chemical stability	Stable under the recommended storage conditions. Moisture-sensitive and light-sensitive.
Possibility of hazardous reactions, including those associated with foreseeable emergencies	No hazardous reactions known under normal processing.
Conditions to avoid (e.g., static discharge, shock, or vibration)	Exposure to light, moist air or water; excess heat; dust formation; contact with incompatible materials.
Incompatible materials	Strong oxidizing agents, strong acids, strong bases.
Hazardous decomposition products	Thermal decomposition can release carbon monoxide, carbon dioxide, nitrogen oxides (NOx), oxides of phosphorus and hydrogen fluoride.

Section 11. Toxicological information

Information on the likely routes of exposure (inhalation, ingestion, skin, and eye contact)	Skin contact, eye contact, inhalation of dust and ingestion.
Symptoms related to the physical, chemical, and toxicological characteristics	Skin: redness, itching and irritation; in sensitized persons, allergic dermatitis (rash, itching, swelling). Eyes: redness, pain, watering and irritation. Inhalation: irritation of the nose, throat and airways (coughing, sneezing, shortness of breath). Ingestion: harmful if swallowed.

Delayed and immediate effects and also chronic effects from short- and long-term exposure	Immediate effects: harmful if swallowed; skin irritation, serious eye irritation and respiratory tract irritation from dust. Delayed effects: allergic skin reaction; repeated or prolonged skin contact may cause allergic reactions in susceptible persons. Once sensitized, a person may react to very small amounts. Chronic effects: no data available on the effects of long-term or repeated exposure.
Numerical measures of toxicity (such as acute toxicity estimates)	Acute oral toxicity: Category 4 (harmful if swallowed); no LD50 value is available. Acute dermal and inhalation toxicity: no data available. No other numerical toxicity data available.
Interactive effects; information on interactions should be included if relevant and readily available	No information available.
Whether the hazardous chemical is listed in the National Toxicology Program (NTP) Report on Carcinogens (latest edition) or has been found to be a potential carcinogen in the International Agency for Research on Cancer (IARC) Monographs (latest edition), or by OSHA	Not listed as a carcinogen or potential carcinogen by NTP (Report on Carcinogens), IARC or OSHA.
When specific chemical data or information is not available, whether alternative information is used and the method used to derive the information (e.g., information from a class of chemicals rather than the exact chemical, using SAR)	No information from analogous substances or chemical classes was used. No study reports for PyBOP itself were found; the classification follows the classifications that suppliers publish for this substance.

Section 12. Ecological information

Ecotoxicity (aquatic and terrestrial, where available)	Very toxic to aquatic life with long lasting effects (aquatic acute 1, chronic 1). No measured ecotoxicity values are available. Do not let the product enter drains, surface water or soil.
Persistence and degradability	No information available.
Bioaccumulative potential	No information available.
Mobility in soil	No information available.
Other adverse effects (such as hazardous to the ozone layer)	No ozone-depleting potential. No other adverse effects known.

Section 13. Disposal considerations

Description of waste residues and information on their safe handling and methods of disposal, including the disposal of any contaminated packaging	Dispose of contents and container as hazardous chemical waste through a licensed waste disposal company, in accordance with local, state and federal regulations. Waste generators must determine whether the discarded material is a hazardous waste under US EPA rules (40 CFR Part 261) and any state rules. Contaminated packaging: dispose of as unused product. Do not dispose of in drains or with household waste. Avoid release to the environment.

Section 14. Transport information

US DOT: not regulated.

IMDG: not offered — P3 does not ship by sea.

IATA: regulated; see 14.a–14.e.

UN number	• IATA: UN3077
UN proper shipping name	• IATA: Environmentally hazardous substance, solid, n.o.s. (benzotriazol-1-yloxytripyrrolidinophosphonium hexafluorophosphate)
Transport hazard class(es)	• IATA: 9
Packing group, if applicable	• IATA: III
Environmental hazards (e.g., Marine pollutant (Yes/No))	• IATA: not a marine pollutant
Transport in bulk (according to IMO instruments)	Not applicable. The product is shipped only in non-bulk packages and is not shipped by sea.
Special precautions which a user needs to be aware of, or needs to comply with, in connection with transport or conveyance either within or outside their premises	Environmentally hazardous substance: if a package is damaged in transit, prevent the contents from entering drains or waterways.

Section 15. Regulatory information

Safety, health and environmental regulations specific for the product in question	TSCA: The chemicals shipped by P3 BioSystems are not subject to TSCA. SARA Title III, Sections 302 and 313: not listed. SARA 311/312 hazard categories: see Section 2. CERCLA: not a listed hazardous substance (no reportable quantity). California Proposition 65: this product does not contain any chemicals known to the State of California to cause cancer, birth defects or other reproductive harm.

Section 16. Other information, including date of preparation or last revision

The date of preparation of the SDS or the last change to it	Date of preparation: 2026-10-07.

The information above is believed to be accurate and represents the best information available to P3 BioSystems on the date of preparation. It is provided for the safe handling of the product by trained persons in a laboratory and is not a warranty of any kind.