

MATERIAL SAFETY DATA SHEET

Section 1 - Identification

Product identifier	PyBOP
Catalog No.	AS2005
Other identifiers	Benzotriazol-1-yloxytripyrrolidinophosphonium hexafluorophosphate; PyBOP
Recommended use	Laboratory research and peptide synthesis; coupling reagent/additive for research-scale synthetic chemistry.
Restrictions on use	For research use only. Not for human or veterinary therapeutic, diagnostic, food, household or consumer applications.
Responsible party	Alan Scientific Inc.
U.S. address	9031 Shady Grove Court, Gaithersburg, MD 20877 U.S.
Contact	+1 888-757-1116 contactus@alanscientific.com www.alanscientific.com
Emergency telephone	+1 888-757-1116

Section 2 - Hazard(s) Identification

OSHA HCS classification	Acute toxicity, oral - Category 4; Skin sensitization - Category 1; Hazardous to the aquatic environment, acute - Category 1; hazardous to the aquatic environment, chronic - Category 1.
Signal word	Warning
Pictograms	GHS07 (Exclamation mark); GHS09 (Environment)
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	Avoid breathing dust. Wash thoroughly after handling. Do not eat, drink or smoke when using this product. Wear protective gloves. Avoid release to the environment. If swallowed, contact a poison center or physician if unwell.
HNOC	None identified beyond the hazards described above based on the reviewed sources.

Section 3 - Composition / Information on Ingredients

Substance / mixture	Substance
Chemical name	Benzotriazol-1-yloxytripyrrolidinophosphonium hexafluorophosphate
CAS No.	128625-52-5
Molecular formula	C18H28F6N6OP2
Molecular weight	520.39 g/mol
Purity / concentration	Product-specific; refer to Certificate of Analysis (COA).

Section 4 - First-Aid Measures

Inhalation: Move to fresh air and keep comfortable for breathing; obtain medical attention if symptoms occur. Skin contact: Remove contaminated clothing and wash with plenty of soap and water; seek medical advice for persistent irritation or allergic reaction. Eye contact: Rinse cautiously with water for at least 15 minutes, remove contact lenses if easy to do, and obtain medical advice if irritation persists. Ingestion: Rinse mouth; do not induce vomiting unless directed by medical personnel; contact a physician or poison center if unwell. Treat symptomatically.

Section 5 - Fire-Fighting Measures

Use water spray, carbon dioxide, dry chemical or chemical foam as appropriate. Prevent contaminated firefighting runoff from entering drains or watercourses. Combustion may generate carbon oxides, nitrogen oxides, phosphorus oxides and hydrogen fluoride.

Section 6 - Accidental Release Measures

Avoid dust formation and inhalation. Remove ignition sources where applicable. Provide adequate ventilation and wear suitable protective equipment. Sweep or collect carefully without generating dust and place in a closed container for disposal. Prevent release to drains and the environment, especially for environmentally hazardous material.

Section 7 - Handling and Storage

Handle using good laboratory practice. Avoid ingestion, inhalation of dust, and contact with skin and eyes. Store tightly closed, dry and cool. Recommended product storage: 2-8 C. Protect from moisture and incompatible materials.

Section 8 - Exposure Controls / Personal Protection

Occupational exposure limits	No substance-specific OSHA PEL or ACGIH TLV identified in the reviewed supplier information.
Engineering controls	Use adequate general ventilation; local exhaust is appropriate where dust may be generated. Provide eyewash and safety shower access.
Eye / face protection	Chemical safety glasses or goggles appropriate to the laboratory task.
Skin / body protection	Suitable chemical-resistant gloves and laboratory clothing. Inspect gloves before use.
Respiratory protection	Normally use engineering controls first. If dust exposure cannot be adequately controlled, use an appropriate NIOSH-approved particulate respirator according to applicable respiratory-protection requirements.
Hygiene measures	Wash thoroughly after handling. Do not eat, drink or smoke in chemical handling areas.

Section 9 - Physical and Chemical Properties

Physical state	Solid / powder
Appearance	Off-white to pale beige powder
Odor	No data available
pH	No data available unless specified by lot or supplier
Melting point / range	Approx. 140-160 C
Boiling point / range	No data available
Flammability	See Section 2 and Section 5
Flash point	No data available / not applicable to supplied solid where indicated
Auto-ignition temperature	No data available
Decomposition temperature	No complete product-specific value available
Vapor pressure	No data available
Density / relative density	No data available
Water solubility	No fixed Alan Scientific specification; refer to product/lot information where provided
Partition coefficient	No data available
Kinematic viscosity	Not applicable to supplied solid
Molecular weight	520.39 g/mol

Section 10 - Stability and Reactivity

Stable under recommended storage conditions based on reviewed supplier documentation. Avoid incompatible materials and excessive heat. Strong oxidizing agents may be incompatible. Thermal decomposition may generate carbon oxides, nitrogen oxides, phosphorus-containing compounds and hydrogen fluoride.

Section 11 - Toxicological Information

Harmful if swallowed and may cause allergic skin reaction based on reviewed U.S. supplier classifications. Other toxicological endpoints are incompletely characterized. Not identified as a listed carcinogen by IARC, NTP or OSHA in the reviewed U.S. supplier documentation.

Section 12 - Ecological Information

Very toxic to aquatic life with long lasting effects. Avoid release to drains, surface water and the environment.

Section 13 - Disposal Considerations

Dispose of contents and contaminated packaging in accordance with applicable federal, state and local requirements. Chemical waste generators are responsible for determining appropriate waste classification. Do not mix with incompatible waste streams. Prevent unnecessary environmental release.

Section 14 - Transport Information

UN number	UN3077
Proper shipping name	Environmentally hazardous substance, solid, n.o.s. (PyBOP)
Hazard class	9
Packing group	III
DOT / IATA / IMDG	Regulated as above based on current supplier transport documentation.

Section 15 - Regulatory Information

This document is prepared for U.S. research-use supply with reference to OSHA Hazard Communication requirements. Public supplier classifications for PyBOP have not been completely uniform; this draft follows current Sigma/Novabiochem hazard classification and corroborating U.S. supplier transport information. Align the final released document with the actual upstream lot-specific safety document when available.

Section 16 - Other Information

Revision	1.0
Date of preparation / revision	2026-09-06
Revision summary	Initial Alan Scientific no-logo MSDS prepared in the current 16-section format for this coupling reagent/additive.
Data / assessment basis	Alan Scientific product information; current Sigma/Novabiochem U.S. product safety information; Thermo Fisher/Acros U.S. SDS revised 2024-01-23; OSHA Hazard Communication Standard.

Safety information notice: The information is provided in good faith for safe handling of the supplied research material and is based on information reasonably available as of the revision date. It is not a product specification or warranty. Users are responsible for determining suitability, controls, transport classification and regulatory obligations for their specific lot, use and jurisdiction.