

# • SAFETY DATA SHEET

Version 6.11  
Revision Date 11/06/2025  
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## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : (Benzotriazol-1-yloxy)tripyrrolidinophosphonium hexafluorophosphate

Product Number : 377848  
Brand : Aldrich  
CAS-No. : 128625-52-5

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

Identified uses : Laboratory chemicals, Synthesis of substances

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 number

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)

#### Hazards for the product as supplied

Acute toxicity (Oral) : Category 4

Skin sensitisation : Category 1

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.  
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:

### SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance  
CAS-No. : 128625-52-5

#### Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
benzotriazol-1-yloxytripyrrolidinophosphonium hexafluorophosphate	128625-52-5*	$\geq 90 - \leq 100$	-

\* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

### SECTION 4. FIRST AID MEASURES

General advice : Hydrofluoric (HF) acid burns require immediate and specialized first aid and medical treatment. Symptoms may be delayed up to 24 hours depending on the concentration of HF. After decontamination with water, further damage can occur due to penetration/absorption of the fluoride ion. Treatment should be directed toward binding the fluoride ion as well as the effects of exposure. Skin exposures can be treated with a 2.5% calcium gluconate gel repeated until burning ceases. More serious skin exposures may require subcutaneous calcium gluconate except for digital areas unless the physician is experienced in this technique, due to the potential for tissue injury from increased pressure. Absorption can readily occur through the subungual areas and should be considered when undergoing decontamination. Prevention of absorption of the fluoride ion in cases of ingestion can be obtained by giving milk, chewable calcium carbonate tablets or Milk of Magnesia to conscious victims. Conditions such as hypocalcemia, hypomagnesemia and cardiac arrhythmias should be monitored for, since they can occur after exposure. Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air.

In case of skin contact	: First treatment with calcium gluconate paste.  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

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## SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO <sub>2</sub> ) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.  Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	: Carbon oxides  Nitrogen oxides (NO <sub>x</sub> )  Oxides of phosphorus  Hydrogen fluoride

Specific extinguishing methods	: No data available
Further information	: Suppress (knock down) gases/vapours/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.

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## 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 precautions	: Do not let product enter drains.
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.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Further information on storage conditions	: Tightly closed. Dry.
Storage class	: 11, Combustible Solids
Recommended storage temperature	: 36 - 46 °F / 2 - 8 °C
Further information on storage stability	: Light sensitive. Moisture sensitive.

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## 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

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](http://www.kcl.de)).

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards

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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.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : solid

Color : No data available

Odor : No data available

Odor Threshold : No data available

pH : No data available

Melting point/ range : 309 - 313 °F / 154 - 156 °C  
Method: dec.

Boiling point/boiling range : No data available

Flash point : No data available

Evaporation rate : No data available

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 vapour density : No data available

Relative density : No data available

Density : 1.438 g/cm<sup>3</sup> (68 °F / 20 °C)  
Method: OECD Test Guideline 109  
GLP: yes

Solubility(ies)

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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

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## 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	: Strong oxidizing agents
Hazardous decomposition products	: In the event of fire: see section 5



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## 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 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.

NTP: No component 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

Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia.  
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.

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## 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

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### **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.

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### **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

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Marine pollutant : yes

### **Transport in bulk according to IMO instruments**

Not applicable for product as supplied.

### **National Regulations**

#### **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.

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## **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 311/312 Hazards** : Acute Health Hazard

**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 components 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.

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## **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 - 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 Harmonised 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 Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; 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 - Organisation 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

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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](http://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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