

## Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

### PRODUCT NAME

(BENZOTRIAZOL-1-YLOXY)TRIPYRROLIDINOPHOSPHONIUM HEXAFLUOROPHOSPHATE

### OTHER NAMES

C18-H28-F6-N6-O-P2, PyBOP

### PRODUCT USE

Coupling reagent for peptide synthesis.  
Intermediate

### SUPPLIER

Company: S D FINE- CHEM LIMITED

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## Section 2 - HAZARDS IDENTIFICATION

### GHS Classification

Chronic Aquatic Hazard Category 3

Eye Irritation Category 2A

Skin Corrosion/Irritation Category 2

STOT - SE Category 3



### EMERGENCY OVERVIEW

#### HAZARD

#### WARNING

Determined by using GHS criteria

|      |                                                    |
|------|----------------------------------------------------|
| H315 | Causes skin irritation.                            |
| H319 | Causes serious eye irritation.                     |
| H335 | May cause respiratory irritation.                  |
| H412 | Harmful to aquatic life with long lasting effects. |

### PRECAUTIONARY STATEMENTS

#### Prevention

| Code | Phrase                                                                     |
|------|----------------------------------------------------------------------------|
| P261 | Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.                     |
| P264 | Wash ... thoroughly after handling.                                        |
| P271 | Use only outdoors or in a well- ventilated area.                           |
| P273 | Avoid release to the environment.                                          |
| P280 | Wear protective gloves/protective clothing/eye protection/face protection. |

#### Response

| Code      | Phrase                                          |
|-----------|-------------------------------------------------|
| P302+P352 | IF ON SKIN: Wash with plenty of soap and water. |

|                      |                                                                                                                                  |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------|
| P304+P340            | IF INHALED: Remove victim to fresh air and keep at rest in a position 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/physician if you feel unwell.                                                                     |
| P332+P313            | If skin irritation occurs: Get medical advice/attention.                                                                         |
| P337+P313            | If eye irritation persists: Get medical advice/attention.                                                                        |
| P362                 | Take off contaminated clothing and wash before re- use.                                                                          |
| <b>Storage Code</b>  | <b>Phrase</b>                                                                                                                    |
| P403+P233            | Store in a well- ventilated place. Keep container tightly closed.                                                                |
| P405                 | Store locked up.                                                                                                                 |
| <b>Disposal Code</b> | <b>Phrase</b>                                                                                                                    |
| P501                 | Dispose of contents/container to ...                                                                                             |

### Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

| NAME                                                         | CAS RN      | %   |
|--------------------------------------------------------------|-------------|-----|
| benzotriazol- 1- yloxypyrrolidinophosphonium fluorophosphate | 128625-52-5 | >98 |

### Section 4 - FIRST AID MEASURES

#### SWALLOWED

- Immediately give a glass of water.
- First aid is not generally required. If in doubt, contact a Poisons Information Centre or a doctor.

#### EYE

- If this product comes in contact with the eyes:
- Wash out immediately with fresh running water.
- Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.
- Seek medical attention without delay; if pain persists or recurs seek medical attention.
- Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.

#### SKIN

- If skin contact occurs:
- Immediately remove all contaminated clothing, including footwear.
- Flush skin and hair with running water (and soap if available).
- Seek medical attention in event of irritation.

#### INHALED

- If fumes or combustion products are inhaled remove from contaminated area.
- Lay patient down. Keep warm and rested.
- Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures.
- Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary.

#### NOTES TO PHYSICIAN

- Treat symptomatically.

### Section 5 - FIRE FIGHTING MEASURES

#### EXTINGUISHING MEDIA

- Foam.
- Dry chemical powder.
- BCF (where regulations permit).
- Carbon dioxide.

#### FIRE FIGHTING

- Alert Fire Brigade and tell them location and nature of hazard.
- Wear breathing apparatus plus protective gloves.
- Prevent, by any means available, spillage from entering drains or water courses.

- Use water delivered as a fine spray to control fire and cool adjacent area.

**FIRE/EXPLOSION HAZARD**

- Combustible solid which burns but propagates flame with difficulty; it is estimated that most organic dusts are combustible (circa 70%) - according to the circumstances under which the combustion process occurs, such materials may cause fires and / or dust explosions.
- Organic powders when finely divided over a range of concentrations regardless of particulate size or shape and suspended in air or some other oxidizing medium may form explosive dust-air mixtures and result in a fire or dust explosion (including secondary explosions).
- Avoid generating dust, particularly clouds of dust in a confined or unventilated space as dusts may form an explosive mixture with air, and any source of ignition, i.e. flame or spark, will cause fire or explosion. Dust clouds generated by the fine grinding of the solid are a particular hazard; accumulations of fine dust (420 micron or less) may burn rapidly and fiercely if ignited - particles exceeding this limit will generally not form flammable dust clouds; once initiated, however, larger particles up to 1400 microns diameter will contribute to the propagation of an explosion.
- In the same way as gases and vapours, dusts in the form of a cloud are only ignitable over a range of concentrations; in principle, the concepts of lower explosive limit (LEL) and upper explosive limit (UEL) are applicable to dust clouds but only the LEL is of practical use; - this is because of the inherent difficulty of achieving homogeneous dust clouds at high temperatures (for dusts the LEL is often called the "Minimum Explosible Concentration", MEC).

Combustion products include: carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>), hydrogen fluoride, nitrogen oxides (NO<sub>x</sub>), phosphorus oxides (PO<sub>x</sub>), other pyrolysis products typical of burning organic material.

May emit poisonous fumes.

May emit corrosive fumes.

**FIRE INCOMPATIBILITY**

- Avoid contamination with oxidising agents i.e. nitrates, oxidising acids, chlorine bleaches, pool chlorine etc. as ignition may result.

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**Section 6 - ACCIDENTAL RELEASE MEASURES**

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**MINOR SPILLS**

- Environmental hazard - contain spillage.
- Clean up all spills immediately.
- Avoid breathing dust and contact with skin and eyes.
- Wear protective clothing, gloves, safety glasses and dust respirator.
- Use dry clean up procedures and avoid generating dust.

**MAJOR SPILLS**

- Environmental hazard - contain spillage.
- Moderate hazard.
- CAUTION: Advise personnel in area.
- Alert Emergency Services and tell them location and nature of hazard.
- Control personal contact by wearing protective clothing.
- Prevent, by any means available, spillage from entering drains or water courses.

**Personal Protective Equipment advice is contained in Section 8 of the MSDS.**

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**Section 7 - HANDLING AND STORAGE**

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**PROCEDURE FOR HANDLING**

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.
- Use in a well-ventilated area.
- Prevent concentration in hollows and sumps.
- Organic powders when finely divided over a range of concentrations regardless of particulate size or shape and suspended in air or some other oxidizing medium may form explosive dust-air mixtures and result in a fire or dust explosion (including secondary explosions)
- Minimise airborne dust and eliminate all ignition sources. Keep away from heat, hot surfaces, sparks, and flame.
- Establish good housekeeping practices.
- Remove dust accumulations on a regular basis by vacuuming or gentle sweeping to avoid creating dust clouds.

**SUITABLE CONTAINER**

- Polyethylene or polypropylene container.
- Check all containers are clearly labelled and free from leaks.

**STORAGE INCOMPATIBILITY**

- Salts of inorganic fluoride:
- react with water forming acidic solutions.

- are violent reactive with boron, bromine pentafluoride, bromine trifluoride, calcium disilicide, calcium hydride, oxygen difluoride, platinum, potassium.
- in aqueous solutions are incompatible with sulfuric acid, alkalis, ammonia, aliphatic amines, alkanolamines, alkylene oxides, amides, epichlorohydrin, isocyanates, nitromethane, organic anhydrides, vinyl acetate.
- corrode metals in presence of moisture.
- Avoid reaction with oxidising agents.

**STORAGE REQUIREMENTS**

- Store in original containers.
  - Keep containers securely sealed.
  - Store in a cool, dry, well-ventilated area.
  - Store away from incompatible materials and foodstuff containers.
- May decompose on exposure to light. Moisture sensitive.

**Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION****EXPOSURE CONTROLS**

| Source                                                                      | Material                                                                      | TWA mg/m <sup>3</sup> |
|-----------------------------------------------------------------------------|-------------------------------------------------------------------------------|-----------------------|
| India Permissible Levels of Certain Chemical Substances in Work Environment | benzotriazol- 1-yloxypyrrolidinophosphonium fluorophosphate (Fluoride (as F)) | 2.5                   |

**MATERIAL DATA****BENZOTRIAZOL-1-YLOXYPYRROLIDINOPHOSPHONIUMFLUOROPHOSPHATE:**

■ It is the goal of the ACGIH (and other Agencies) to recommend TLVs (or their equivalent) for all substances for which there is evidence of health effects at airborne concentrations encountered in the workplace. At this time no TLV has been established, even though this material may produce adverse health effects (as evidenced in animal experiments or clinical experience).

NOTE: The ACGIH occupational exposure standard for Particles Not Otherwise Specified (P.N.O.S) does NOT apply.

Sensory irritants are chemicals that produce temporary and undesirable side-effects on the eyes, nose or throat. Historically occupational exposure standards for these irritants have been based on observation of workers' responses to various airborne concentrations.

For fluorides:

Based on a study in which the threshold for minimum increase in bone density due to fluoride exposure was 3.38 mg/m<sup>3</sup> (as fluoride), the present TLV-TWA has been adopted to prevent irritant effects and disabling bone changes. There is also support for the proposition that occupational exposure below the TLV will have no adverse effect on pregnant women or off-spring.

**PERSONAL PROTECTION****RESPIRATOR**

- Particulate. (AS/NZS 1716 & 1715, EN 143:2000 & 149:2001, ANSI Z88 or national equivalent)

**EYE**

- Safety glasses with side shields.
- Chemical goggles.
- Contact lenses may pose a special hazard; soft contact lenses may absorb and concentrate irritants. A written policy document, describing the wearing of lens or restrictions on use, should be created for each workplace or task. This should include a review of lens absorption and adsorption for the class of chemicals in use and an account of injury experience. Medical and first-aid personnel should be trained in their removal and suitable equipment should be readily available. In the event of chemical exposure, begin eye irrigation immediately and remove contact lens as soon as practicable. Lens should be removed at the first signs of eye redness or irritation - lens should be removed in a clean environment only after workers have washed hands thoroughly. [CDC NIOSH Current Intelligence Bulletin 59], [AS/NZS 1336 or national equivalent].

**HANDS/FEET**

■ The selection of the suitable gloves does not only depend on the material, but also on further marks of quality which vary from manufacturer to manufacturer. Where the chemical is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.

The exact break through time for substances has to be obtained from the manufacturer of the protective gloves and has to be observed when making a final choice.

Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include:.

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**Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION**

Experience indicates that the following polymers are suitable as glove materials for protection against undissolved, dry solids, where abrasive particles are not present.

- polychloroprene
- nitrile rubber
- butyl rubber
- fluorocautchouc.

**OTHER**

- Overalls.
- P.V.C. apron.
- Barrier cream.
- Skin cleansing cream.

**ENGINEERING CONTROLS**

■ Engineering controls are used to remove a hazard or place a barrier between the worker and the hazard. Well-designed engineering controls can be highly effective in protecting workers and will typically be independent of worker interactions to provide this high level of protection.

The basic types of engineering controls are:

Process controls which involve changing the way a job activity or process is done to reduce the risk.

Enclosure and/or isolation of emission source which keeps a selected hazard "physically" away from the worker and ventilation that strategically "adds" and "removes" air in the work environment.

**Section 9 - PHYSICAL AND CHEMICAL PROPERTIES****APPEARANCE**

White powder; does not mix well with water. Soluble in acetonitrile.

**PHYSICAL PROPERTIES**

Solid.

Does not mix with water.

|                           |                  |                                 |                 |
|---------------------------|------------------|---------------------------------|-----------------|
| State                     | Divided solid    | Molecular Weight                | 520.40          |
| Melting Range (°C)        | 154- 156(decomp) | Viscosity                       | Not Applicable  |
| Boiling Range (°C)        | Not applicable   | Solubility in water (g/L)       | Partly miscible |
| Flash Point (°C)          | Not available    | pH (1% solution)                | Not applicable  |
| Decomposition Temp (°C)   | 154              | pH (as supplied)                | Not applicable  |
| Autoignition Temp (°C)    | Not available    | Vapour Pressure (kPa)           | Negligible      |
| Upper Explosive Limit (%) | Not available.   | Specific Gravity (water=1)      | Not available   |
| Lower Explosive Limit (%) | Not available    | Relative Vapour Density (air=1) | Not Applicable  |
| Volatile Component (%vol) | Negligible       | Evaporation Rate                | Not applicable  |

**Section 10 - CHEMICAL STABILITY AND REACTIVITY INFORMATION****CONDITIONS CONTRIBUTING TO INSTABILITY**

- Presence of incompatible materials.
- Product is considered stable.
- Hazardous polymerisation will not occur.

For incompatible materials - refer to Section 7 - Handling and Storage.

**Section 11 - TOXICOLOGICAL INFORMATION****Health hazard summary table:**

|                                   |                |
|-----------------------------------|----------------|
| Acute toxicity                    | Not applicable |
| Skin corrosion/irritation         | Skin Irrit. 2  |
| Serious eye damage/irritation     | Eye Irrit. 2A  |
| Respiratory or skin sensitization | Not applicable |
| Germ cell mutagenicity            | Not applicable |
| Carcinogenicity                   | Not applicable |
| Reproductive toxicity             | Not applicable |
| STOT- single exposure             | STOT SE 3      |
| STOT- repeated exposure           | Not applicable |
| Aspiration hazard                 | Not applicable |

continued...

**POTENTIAL HEALTH EFFECTS****ACUTE HEALTH EFFECTS****SWALLOWED**

- The material has NOT been classified by EC Directives or other classification systems as "harmful by ingestion". This is because of the lack of corroborating animal or human evidence.

**EYE**

- This material can cause eye irritation and damage in some persons.

**SKIN**

- This material can cause inflammation of the skin on contact in some persons.
- The material may accentuate any pre-existing dermatitis condition.
- Skin contact is not thought to have harmful health effects (as classified under EC Directives); the material may still produce health damage following entry through wounds, lesions or abrasions.
- Open cuts, abraded or irritated skin should not be exposed to this material.
- Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects. Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

**INHALED**

- The material can cause respiratory irritation in some persons. The body's response to such irritation can cause further lung damage.
- Persons with impaired respiratory function, airway diseases and conditions such as emphysema or chronic bronchitis, may incur further disability if excessive concentrations of particulate are inhaled. If prior damage to the circulatory or nervous systems has occurred or if kidney damage has been sustained, proper screenings should be conducted on individuals who may be exposed to further risk if handling and use of the material result in excessive exposures.
- Acute effects of fluoride inhalation include irritation of nose and throat, coughing and chest discomfort. A single acute over-exposure may even cause nose bleed.

**CHRONIC HEALTH EFFECTS**

- Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems. Substance accumulation, in the human body, may occur and may cause some concern following repeated or long-term occupational exposure. Long term exposure to high dust concentrations may cause changes in lung function i.e. pneumoconiosis; caused by particles less than 0.5 micron penetrating and remaining in the lung. Prime symptom is breathlessness; lung shadows show on X-ray. Extended exposure to inorganic fluorides causes fluorosis, which includes signs of joint pain and stiffness, tooth discolouration, nausea and vomiting, loss of appetite, diarrhoea or constipation, weight loss, anaemia, weakness and general unwellness. There may also be frequent urination and thirst. Redness, itchiness and allergy-like inflammation of the skin and mouth cavity can occur. The central nervous system may be involved.

**TOXICITY AND IRRITATION**

- Asthma-like symptoms may continue for months or even years after exposure to the material ceases. This may be due to a non-allergenic condition known as reactive airways dysfunction syndrome (RADS) which can occur following exposure to high levels of highly irritating compound. No significant acute toxicological data identified in literature search.

**Section 12 - ECOLOGICAL INFORMATION**

May cause long-term adverse effects in the environment.  
Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.  
Toxic to soil organisms.

**Ecotoxicity**

| Ingredient                                                          | Persistence:<br>Water/Soil | Persistence: Air     | Bioaccumulation      | Mobility             |
|---------------------------------------------------------------------|----------------------------|----------------------|----------------------|----------------------|
| benzotriazol- 1-<br>yloxy pyrrolidinophosphonium<br>fluorophosphate | No Data<br>Available       | No Data<br>Available | No Data<br>Available | No Data<br>Available |

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## Section 13 - DISPOSAL CONSIDERATIONS

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■ Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area.

A Hierarchy of Controls seems to be common - the user should investigate:

- Reduction.
- DO NOT allow wash water from cleaning or process equipment to enter drains.
- It may be necessary to collect all wash water for treatment before disposal.
- In all cases disposal to sewer may be subject to local laws and regulations and these should be considered first.
- Where in doubt contact the responsible authority.

For small quantities:

- Cautiously dissolve in water
- Neutralise with sodium carbonate or if product does not dissolve completely add a small quantity of hydrochloric acid followed by sodium carbonate
- Add excess calcium chloride to precipitate the fluoride and/ or carbonate
- Remove solids to site approved for hazardous waste.
- Recycle wherever possible.
- Consult manufacturer for recycling options or consult local or regional waste management authority for disposal if no suitable treatment or disposal facility can be identified.
- Dispose of by: burial in a land-fill specifically licenced to accept chemical and / or pharmaceutical wastes or Incineration in a licenced apparatus (after admixture with suitable combustible material)
- Decontaminate empty containers. Observe all label safeguards until containers are cleaned and destroyed.

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## Section 14 - TRANSPORTATION INFORMATION

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### HAZCHEM:

None

NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS: UN, IATA, IMDG

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## Section 15 - REGULATORY INFORMATION

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## Section 16 - OTHER INFORMATION

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