Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent)

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830

Date of issue: 8/19/2019 Version: 1.0

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product form	: Substance
Substance name	: Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent)
IUPAC name	: (1H-benzotriazol-1-yloxy)[tris(dimethylamino)]phosphonium hexafluorophosphate
EC-No.	: 260-279-1
CAS-No.	: 56602-33-6
Product code	: 45328655
Formula	: C12H22F6N6OP2
Product group	: Raw material

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

1.2.1. Relevant identified uses

Main use category	: Laboratory use,Industrial use,Professional use
Industrial/Professional use spec	: For professional use only
Use of the substance/mixture	: For analytical purposes Scientific research and development Not for human consumption or veterinary purposes.

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Supplier

Scafell Organics
Molekula Ltd
Lingfield Way
Darlington - England
T +44 (0) 1949 823777 / +44 (0) 7590 545705
info@molekula.com / kbowen@molekula.com - www.molekula.com

1.4. Emergency telephone number

Emergency number : +44 (0) 7590 545705

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Flammable solids, Category 2	H228
Skin corrosion/irritation, Category 2	H315
Serious eye damage/eye irritation, Category 2	H319
Specific target organ toxicity — Single exposure, Category 3, Respiratory tract irritation	H335

Full text of H statements : see section 16

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS02 GHS07

Signal word (CLP) : Warning

Hazard statements (CLP) : H228 - Flammable solid.
H315 - Causes skin irritation.
H319 - Causes serious eye irritation.
H335 - May cause respiratory irritation.

Precautionary statements (CLP)	: P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P220 - Keep away from clothing and other combustible materials. P261 - Avoid breathing dust/fume/gas/mist/vapours/spray. P280 - Wear protective gloves/protective clothing/eye protection/face protection. P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

2.3. Other hazards

This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII

This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

SECTION 3: Composition/information on ingredients

3.1. Substances

Name	Product identifier	%
Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent)	(CAS-No.) 56602-33-6 (EC-No.) 260-279-1	100

Full text of H-statements: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: If possible show this sheet, if not available show packaging or label. Never give anything by mouth to an unconscious person. Do not leave affected person unattended.
First-aid measures after inhalation	: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing. Give oxygen or artificial respiration if necessary. If breathing difficulties persist : Get medical advice/attention.
First-aid measures after skin contact	: After contact with skin, take off immediately all contaminated clothing, and wash immediately with plenty of water. Do not remove clothing if it sticks to the skin. If irritation persists, consult a doctor.
First-aid measures after eye contact	: Rinse immediately with plenty of water. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
First-aid measures after ingestion	: Rinse mouth out with water. Do not induce vomiting. Get medical advice/attention.

4.2. Most important symptoms and effects, both acute and delayed

Symptoms/effects after inhalation	: Inhalation may cause irritation (cough, short breathing, difficulty in breathing).
Symptoms/effects after skin contact	: Causes skin irritation. May cause moderate irritation, including burning sensation, tearing, redness or swelling.
Symptoms/effects after eye contact	: Causes serious eye irritation. redness, itching, tears. stinging.
Symptoms/effects after ingestion	: Ingestion may cause nausea and vomiting.

4.3. Indication of any immediate medical attention and special treatment needed

Get immediate medical advice/attention.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	: Dry powder. Sand.
Unsuitable extinguishing media	: Do NOT use water jet.

5.2. Special hazards arising from the substance or mixture

Fire hazard	: Flammable solid.
Explosion hazard	: May form flammable/explosive vapour-air mixture.
Hazardous decomposition products in case of fire	: Carbon oxides (CO, CO2). hydrogen fluoride. Nitrogen oxides. Phosphorus oxides.

5.3. Advice for firefighters

Precautionary measures fire	: Exposure to fire/heat: seal off low-lying areas. Keep container tightly closed and away from heat, sparks and flame. Keep away from combustible materials.
Firefighting instructions	: Evacuate area. Eliminate all ignition sources if safe to do so. Fight fire from safe distance and protected location. Keep upwind.
Protection during firefighting	: Do not attempt to take action without suitable protective equipment. Use self-contained breathing apparatus and chemically protective clothing.
Other information	: Warn all persons of toxic hazard.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Do not handle until all safety precautions have been read and understood. Ventilate the area thoroughly, especially low lying areas (basements, workpits etc). Proper grounding procedures to avoid static electricity should be followed.

6.1.1. For non-emergency personnel

Protective equipment : Wear recommended personal protective equipment.

Emergency procedures : Evacuate unnecessary personnel. Mark out the contaminated area with signs and prevent access to unauthorized personnel. Do not touch or walk on the spilled product. Avoid contact with skin, eyes and clothing.

Measures in case of dust release : Keep upwind. Avoid creating or spreading dust. Ventilate the area thoroughly, especially low lying areas (basements, workpits etc). Special attention should be given to low areas/pits where flammable vapours can accumulate.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. Use self-contained breathing apparatus and chemically protective clothing.

Emergency procedures : All equipment used when handling the product must be grounded. Prevent from entering sewers, basements and workpits, or any place where its accumulation can be dangerous. Stop leak if safe to do so.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if product enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : On land, sweep or shovel into suitable containers. Shovel or sweep up and put in a closed container for disposal.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Avoid formation of dust. Avoid contact with skin, eyes and clothing. Do not handle until all safety precautions have been read and understood. Ensure that there is a suitable ventilation system. Do not handle in a confined space.

Hygiene measures : Take off immediately all contaminated clothing and wash it before reuse. Contaminated work clothing should not be allowed out of the workplace. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Do not eat, drink or smoke when using this product.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Ensure adequate ventilation, especially in confined areas. Proper grounding procedures to avoid static electricity should be followed.

Storage conditions : Keep only in the original container in a cool, well ventilated place away from : Heat sources, Direct sunlight. Keep container closed when not in use. Light sensitive. Moisture sensitive. Store contents under inert gas.

Incompatible products : Strong oxidizing agents.

Incompatible materials : Sources of ignition. Direct sunlight. Heat sources. open flames. sparks. Light sensitive. Moisture. Water, humidity.

Storage temperature : 2 - 8 °C

Heat and ignition sources : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Storage area : Keep away from combustible materials. Store in dry protected location to prevent any moisture contact. Store in a dark area.

7.3. Specific end use(s)

For analytical purposes. Scientific research and development. Not for human consumption or veterinary purposes.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Appropriate engineering controls:

Handle in accordance with good industrial hygiene and safety procedures.

Personal protective equipment:

Avoid all unnecessary exposure.

Materials for protective clothing:

Wear suitable protective clothing, gloves and eye/face protection

Hand protection:

The protective gloves to be used must comply with the specifications of the regulation 2016/425 and the resultant standard EN 374

Type	Material	Permeation	Thickness (mm)	Penetration	Standard
Disposable gloves	Nitrile rubber (NBR)	6 (> 480 minutes)	0.11		EN 374

Eye protection:

Emergency eye wash fountains should be available in the immediate vicinity of any potential exposure. Use eye protection according to EN 166, designed to protect against powders and dusts.

Type	Use	Characteristics	Standard
Safety goggles, Face shield	Fine dust, Dust	tightly fitting safety goggles, With side shields	EN 166

Skin and body protection:

Emergency safety showers should be available in the immediate vicinity of any potential exposure. Keep suitable chemically resistant protective clothing readily available for emergency use

Type	Standard
Total impervious protective suits, gloves, and boots must be worn to prevent any contact with the product, Flame retardant antistatic protective clothing	EN ISO 13982

Respiratory protection:

Keep self contained breathing apparatus readily available for emergency use. Where exposure through inhalation may occur from use, respiratory protection equipment is recommended

Device	Filter type	Condition	Standard
Respiratory protective device with a particle filter	Type P3	Dust protection	EN 14387

Other information:

Do not eat, drink or smoke during use.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Solid
Appearance	: Crystalline powder.
Molecular mass	: 442.28 g/mol
Colour	: white.
Odour	: No data available.
Odour threshold	: No data available
pH	: No data available
Relative evaporation rate (butylacetate=1)	: No data available
Melting point	: > 130 °C
Freezing point	: No data available
Boiling point	: No data available
Flash point	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: Flammable
Vapour pressure	: No data available
Relative vapour density at 20 °C	: No data available
Relative density	: No data available
Solubility	: No data available
Log Pow	: No data available
Viscosity, kinematic	: No data available

Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidising properties	: No data available
Explosive limits	: No data available

9.2. Other information
No additional information available

SECTION 10: Stability and reactivity
10.1. Reactivity
Flammable solid.
10.2. Chemical stability
Flammable solid. In use may form flammable/explosive vapour-air mixture.
10.3. Possibility of hazardous reactions
Stable under normal conditions of use.
10.4. Conditions to avoid
Protect from sunlight. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Light sensitive. Moisture. Water, humidity.
10.5. Incompatible materials
Strong oxidizers.
10.6. Hazardous decomposition products
No hazardous decomposition products known at room temperature. Thermal decomposition generates : Carbon oxides (CO, CO2). hydrogen fluoride. Nitrogen oxides. Phosphorus oxides.

SECTION 11: Toxicological information
11.1. Information on toxicological effects
Acute toxicity (oral)	: Not classified
Acute toxicity (dermal)	: Not classified
Acute toxicity (inhalation)	: Not classified
Skin corrosion/irritation	: Causes skin irritation.
Additional information	: Based on available data, the classification criteria are not met
Serious eye damage/irritation	: Causes serious eye irritation.
Additional information	: Based on available data, the classification criteria are not met
Respiratory or skin sensitisation	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Germ cell mutagenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Carcinogenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Reproductive toxicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-single exposure	: May cause respiratory irritation.
Additional information	: Based on available data, the classification criteria are not met
STOT-repeated exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Aspiration hazard	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Potential adverse human health effects and symptoms	: Based on available data, the classification criteria are not met.

SECTION 12: Ecological information
12.1. Toxicity
Acute aquatic toxicity	: Not classified
Chronic aquatic toxicity	: Not classified

12.2. Persistence and degradability
Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent) (56602-33-6)	
Persistence and degradability	No data available.

12.3. Bioaccumulative potential

Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent) (56602-33-6)	
Bioaccumulative potential	No data available.

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent) (56602-33-6)
This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII
This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

12.6. Other adverse effects

Additional information : Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product/Packaging disposal recommendations : Dispose in a safe manner in accordance with local/national regulations.

Additional information : Handle empty containers with care because residual vapours are flammable.

Ecology - waste materials : Avoid release to the environment.

SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

ADR	IMDG	IATA	ADN	RID
14.1. UN number				
1325	1325	1325	1325	1325
14.2. UN proper shipping name				
FLAMMABLE SOLID, ORGANIC, N.O.S.	FLAMMABLE SOLID, ORGANIC, N.O.S.	Flammable solid, organic, n.o.s.	FLAMMABLE SOLID, ORGANIC, N.O.S.	FLAMMABLE SOLID, ORGANIC, N.O.S.
Transport document description				
UN 1325 FLAMMABLE SOLID, ORGANIC, N.O.S. (Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent)), 4.1, II, (E)	UN 1325 FLAMMABLE SOLID, ORGANIC, N.O.S. (Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent)), 4.1, II	UN 1325 Flammable solid, organic, n.o.s. (Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent)), 4.1, II	UN 1325 FLAMMABLE SOLID, ORGANIC, N.O.S. (Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent)), 4.1, II	UN 1325 FLAMMABLE SOLID, ORGANIC, N.O.S. (Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent)), 4.1, II
14.3. Transport hazard class(es)				
4.1	4.1	4.1	4.1	4.1
				
14.4. Packing group				
II	II	II	II	II
14.5. Environmental hazards				
Dangerous for the environment : No	Dangerous for the environment : No Marine pollutant : No	Dangerous for the environment : No	Dangerous for the environment : No	Dangerous for the environment : No
No supplementary information available				

14.6. Special precautions for user

Overland transport

Classification code (ADR) : F1

Special provisions (ADR) : 274

Limited quantities (ADR) : 1kg

Excepted quantities (ADR) : E2

Packing instructions (ADR)	: P002, IBC08
Special packing provisions (ADR)	: B4
Mixed packing provisions (ADR)	: MP10
Portable tank and bulk container instructions (ADR)	: T3
Portable tank and bulk container special provisions (ADR)	: TP33
Tank code (ADR)	: SGAN
Vehicle for tank carriage	: AT
Transport category (ADR)	: 2
Special provisions for carriage - Packages (ADR)	: V11
Hazard identification number (Kemler No.)	: 40
Orange plates	: 
Tunnel restriction code (ADR)	: E
EAC code	: 1Z

Transport by sea

Special provisions (IMDG)	: 274, 915
Limited quantities (IMDG)	: 1 kg
Excepted quantities (IMDG)	: E2
Packing instructions (IMDG)	: P002
IBC packing instructions (IMDG)	: IBC08
IBC special provisions (IMDG)	: B21, B4
Tank instructions (IMDG)	: T3
Tank special provisions (IMDG)	: TP33
EmS-No. (Fire)	: F-A
EmS-No. (Spillage)	: S-G
Stowage category (IMDG)	: B

Air transport

PCA Excepted quantities (IATA)	: E2
PCA Limited quantities (IATA)	: Y441
PCA limited quantity max net quantity (IATA)	: 5kg
PCA packing instructions (IATA)	: 445
PCA max net quantity (IATA)	: 15kg
CAO packing instructions (IATA)	: 448
CAO max net quantity (IATA)	: 50kg
Special provisions (IATA)	: A3, A803
ERG code (IATA)	: 3L

Inland waterway transport

Classification code (ADN)	: F1
Special provisions (ADN)	: 274
Limited quantities (ADN)	: 1 kg
Excepted quantities (ADN)	: E2
Equipment required (ADN)	: PP
Number of blue cones/lights (ADN)	: 1

Rail transport

Classification code (RID)	: F1
Special provisions (RID)	: 274
Excepted quantities (RID)	: E2
Packing instructions (RID)	: P002, IBC08
Special packing provisions (RID)	: B4
Mixed packing provisions (RID)	: MP10
Portable tank and bulk container instructions (RID)	: T3
Portable tank and bulk container special provisions (RID)	: TP33

Tank codes for RID tanks (RID)	: SGAN
Transport category (RID)	: 2
Special provisions for carriage – Packages (RID)	: W1
Colis express (express parcels) (RID)	: CE10
Hazard identification number (RID)	: 40

14.7. Transport in bulk according to Annex II of Marpol and the IBC Code
Not applicable

SECTION 15: Regulatory information
15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture
15.1.1. EU-Regulations

No REACH Annex XVII restrictions
Benzotriazol-1-yl-oxy-tris(dimethylamino) phosphonium hexafluorophosphate (BOP Reagent) is not on the REACH Candidate List
Directive 2012/18/EU (SEVESO III)

15.1.2. National regulations
No additional information available

15.2. Chemical safety assessment
No chemical safety assessment has been carried out for the substance or the mixture by the supplier

SECTION 16: Other information
Data sources : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

Other information : None.

Full text of H- and EUH-statements:	
Eye Irrit. 2	Serious eye damage/eye irritation, Category 2
Flam. Sol. 2	Flammable solids, Category 2
Skin Irrit. 2	Skin corrosion/irritation, Category 2
STOT SE 3	Specific target organ toxicity — Single exposure, Category 3, Respiratory tract irritation
H228	Flammable solid.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

SDS EU (REACH Annex II)
This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.