



SAFETY DATA SHEET

TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate)

According to the REACH etc. (Amendment etc.) (EU Exit) Regulations 2020 No. 1577, as amended.

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

1.1. Product identifier

Product name	TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate)
Chemical name	2-(1H-Benzotriazole-1-yl)-1,1,3,3-tetramethylaminium tetrafluoroborate,
Synonyms; trade names	TBTU, o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate, 1H-Benzotriazolium, 1-[bis(dimethylamino)methylene]-3-oxide tetrafluoroborate
CAS number	125700-67-6
EC number	423-040-4

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

Identified uses	Research and development.
Uses advised against	No specific uses advised against are identified.

1.3. Details of the supplier of the safety data sheet

Supplier	Molekula Ltd. Lingfield Way, Darlington, DL1 4XX, United Kingdom +44 (0) 3302000333 info@molekula.com
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1.4. Emergency telephone number

+44 (0) 7769276927

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (SI 2019 No. 720)

Physical hazards	Flam. Sol. 1 - H228
Health hazards	Acute Tox. 4 - H302 Skin Irrit. 2 - H315 Eye Irrit. 2 - H319 STOT SE 3 - H335
Environmental hazards	Not Classified

2.2. Label elements

EC number	423-040-4
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Hazard pictograms



Signal word	Danger
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TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate)

Hazard statements	H228 Flammable solid. H302 Harmful if swallowed. H315 Causes skin irritation. H319 Causes serious eye irritation. H335 May cause respiratory irritation.
Precautionary statements	P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P240 Ground and bond container and receiving equipment. P241 Use explosion-proof electrical equipment. P261 Avoid breathing dust. P264 Wash contaminated skin thoroughly after handling. P271 Use only outdoors or in a well-ventilated area. P280 Wear protective gloves/ protective clothing/ eye protection/ face protection. P301+P312 IF SWALLOWED: Call a POISON CENTRE/doctor if you feel unwell. P302+P352 IF ON SKIN: Wash with plenty of 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. P330 Rinse mouth. P332+P313 If skin irritation 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. P403+P233 Store in a well-ventilated place. Keep container tightly closed. P405 Store locked up. P501 Dispose of contents/ container in accordance with national regulations.

2.3. Other hazards

This substance is not classified as PBT or vPvB according to current UK criteria.

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate)
Chemical name	2-(1H-Benzotriazole-1-yl)-1,1,3,3-tetramethylaminium tetrafluoroborate,
CAS number	125700-67-6
EC number	423-040-4
Chemical formula	C ₆ H ₄ N ₃ (O)(N(CH ₃) ₂) ₂ . BF ₄

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	Get medical attention if any discomfort continues. Show this Safety Data Sheet to the medical personnel.
Inhalation	Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Maintain an open airway. Loosen tight clothing such as collar, tie or belt. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. Get medical attention. Place unconscious person on their side in the recovery position and ensure breathing can take place.

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Ingestion	Rinse mouth thoroughly with water. Give a few small glasses of water or milk to drink. Stop if the affected person feels sick as vomiting may be dangerous. Never give anything by mouth to an unconscious person. Place unconscious person on their side in the recovery position and ensure breathing can take place. Keep affected person under observation. Get medical attention if symptoms are severe or persist.
Skin contact	Rinse with water.
Eye contact	Rinse with water. Do not rub eye. Remove any contact lenses and open eyelids wide apart. Get medical attention if any discomfort continues.
Protection of first aiders	First aid personnel should wear appropriate protective equipment during any rescue.

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

General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Irritation of nose, throat and airway. Difficulty in breathing. Coughing.
Ingestion	May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.
Skin contact	Redness. Irritating to skin.
Eye contact	Irritating to eyes.

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

Notes for the doctor	Treat symptomatically.
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SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	The product is flammable. Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.
Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.

5.2. Special hazards arising from the substance or mixture

Specific hazards	Flammable solid. Dust may form explosive mixture with air. Fire-water run-off in sewers may create fire or explosion hazard. This product is toxic.
Hazardous combustion products	Thermal decomposition or combustion products may include the following substances: Toxic gases or vapours.

5.3. Advice for firefighters

Protective actions during firefighting	Avoid breathing fire gases or vapours. Evacuate area. Keep upwind to avoid inhalation of gases, vapours, fumes and smoke. Ventilate closed spaces before entering them. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities.
Special protective equipment for firefighters	Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

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Personal precautions Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Evacuate area. Provide adequate ventilation. No smoking, sparks, flames or other sources of ignition near spillage. Promptly remove any clothing that becomes contaminated. Avoid inhalation of dust. Use suitable respiratory protection if ventilation is inadequate.

6.2. Environmental precautions

Environmental precautions Avoid discharge into drains or watercourses or onto the ground. Avoid discharge to the aquatic environment.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Eliminate all ignition sources if safe to do so. No smoking, sparks, flames or other sources of ignition near spillage. Do not allow material to enter confined spaces, due to the risk of explosion. Provide adequate ventilation. Collect spillage with a shovel and broom, or similar and reuse, if possible. Collect and place in suitable waste disposal containers and seal securely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. For waste disposal, see Section 13.

6.4. Reference to other sections

Reference to other sections For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Keep container tightly sealed when not in use. The product is flammable. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not reuse empty containers.

Advice on general occupational hygiene Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions Store away from incompatible materials (see Section 10). Store locked up. Keep away from oxidising materials, heat and flames. Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage.

Moisture sensitive. Store under inert gas.

Storage class Other explosive hazardous substances

7.3. Specific end use(s)

Specific end use(s) The identified uses for this product are detailed in Section 1.2.

SECTION 8: Exposure controls/Personal protection

8.1. Control parameters

8.2. Exposure controls

TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate)

Protective equipment



Appropriate engineering controls

Provide adequate general and local exhaust ventilation. Ensure the ventilation system is regularly maintained and tested. Good general ventilation should be adequate to control worker exposure to airborne contaminants. Observe any occupational exposure limits for the product or ingredients.

Eye/face protection

Wear tight-fitting, chemical splash goggles or face shield. If inhalation hazards exist, a full-face respirator may be required instead.

Hand protection

Wear protective gloves. The most suitable glove should be chosen in consultation with the glove supplier/manufacturer, who can provide information about the breakthrough time of the glove material. To protect hands from chemicals, wear gloves that are proven to be impervious to the chemical and resist degradation. Considering the data specified by the glove manufacturer, check during use that the gloves are retaining their protective properties and change them as soon as any deterioration is detected. Frequent changes are recommended.

Other skin and body protection

Wear appropriate clothing to prevent repeated or prolonged skin contact.

Hygiene measures

Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.

Respiratory protection

Ensure all respiratory protective equipment is suitable for its intended use and is 'UKCA'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges suitable for intended use should be used. Full face mask respirators with replaceable filter cartridges suitable for intended use should be used. Half mask and quarter mask respirators with replaceable filter cartridges suitable for intended use should be used.

Environmental exposure controls

Keep container tightly sealed when not in use. Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	Solid.
Colour	White/off-white.
Odour	Not known.
Odour threshold	No information available.
pH	No information available.
Melting point	195 - 205°C/383 - 401°F
Initial boiling point and range	No information available.
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.

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Upper/lower flammability or explosive limits	No information available.
Vapour pressure	No information available.
Vapour density	No information available.
Relative density	No information available.
Solubility(ies)	No information available.
Partition coefficient	No information available.
Auto-ignition temperature	No information available.
Decomposition Temperature	No information available.

9.2. Other information

Molecular weight	309.07
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SECTION 10: Stability and reactivity

10.1. Reactivity

Reactivity	This is a combustible organic substance. The risk of a dust explosion may be assumed when the substance is finely distributed.
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10.2. Chemical stability

Stability	Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions. Protect from moisture.
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10.3. Possibility of hazardous reactions

Possibility of hazardous reactions	Violent reactions possible with: Strong oxidising agents. Strong alkalis.
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10.4. Conditions to avoid

Conditions to avoid	Avoid generation and spreading of dust. Avoid dust close to ignition sources. Heating (explosive decomposition) Sensitive to Moisture
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10.5. Incompatible materials

Materials to avoid	Avoid contact with strong oxidising agents. Strong alkalis.
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10.6. Hazardous decomposition products

Hazardous decomposition products	Does not decompose when used and stored as recommended. Thermal decomposition or combustion products may include the following substances: Toxic gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO ₂). Nitrous gases (NO _x). Hydrogen fluoride (HF). Oxides of the following substances: Boron.
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SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

Summary	Harmful if swallowed.
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ATE oral (mg/kg)	500.0
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Acute toxicity - dermal

Summary	Based on available data the classification criteria are not met.
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Acute toxicity - inhalation

TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate)

Summary	Based on available data the classification criteria are not met.
<u>Skin corrosion/irritation</u>	
Summary	Causes skin irritation.
<u>Serious eye damage/irritation</u>	
Summary	Causes serious eye irritation.
<u>Respiratory sensitisation</u>	
Summary	Based on available data the classification criteria are not met.
<u>Skin sensitisation</u>	
Summary	Based on available data the classification criteria are not met.
<u>Germ cell mutagenicity</u>	
Summary	Based on available data the classification criteria are not met.
<u>Carcinogenicity</u>	
Summary	Based on available data the classification criteria are not met.
IARC carcinogenicity	None of the ingredients are listed or exempt.
<u>Reproductive toxicity</u>	
Summary	Based on available data the classification criteria are not met.
<u>Specific target organ toxicity - single exposure</u>	
Summary	May cause respiratory irritation.
Target organs	Respiratory system, lungs
<u>Specific target organ toxicity - repeated exposure</u>	
Summary	Based on available data the classification criteria are not met.
<u>Aspiration hazard</u>	
Summary	Not relevant. Solid.
General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Irritation of nose, throat and airway. Difficulty in breathing. Coughing.
Ingestion	May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.
Skin contact	Redness. Irritating to skin.
Eye contact	Irritating to eyes.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	Respiratory system, lungs

SECTION 12: Ecological information

Ecotoxicity	Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.
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12.1. Toxicity

Acute aquatic toxicity

Summary	Based on available data the classification criteria are not met.
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TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate)

Chronic aquatic toxicity

Summary Based on available data the classification criteria are not met.

12.2. Persistence and degradability

Persistence and degradability The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential No data available on bioaccumulation.

Partition coefficient No information available.

12.4. Mobility in soil

Mobility No data available.

12.5. Results of PBT and vPvB assessment

12.6. Other adverse effects

Other adverse effects None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous.

Disposal methods Do not empty into drains. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents. Incineration or landfill should only be considered when recycling is not feasible.

SECTION 14: Transport information

General For limited quantity packaging/limited load information, consult the relevant modal documentation using the data shown in this section.

14.1. UN number

UN No. (ADR/RID) 1325

UN No. (IMDG) 1325

UN No. (ICAO) 1325

UN No. (ADN) 1325

14.2. UN proper shipping name

Proper shipping name (ADR/RID) FLAMMABLE SOLID, ORGANIC, N.O.S. (TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate))

Proper shipping name (IMDG) FLAMMABLE SOLID, ORGANIC, N.O.S. (TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate))

Proper shipping name (ICAO) FLAMMABLE SOLID, ORGANIC, N.O.S. (TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate))

TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate)

Proper shipping name (ADN) FLAMMABLE SOLID, ORGANIC, N.O.S. (TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate))

14.3. Transport hazard class(es)

ADR/RID class	4.1
ADR/RID classification code	F1
ADR/RID label	4.1
IMDG class	4.1
ICAO class/division	4.1
ADN class	4.1

Transport labels



14.4. Packing group

ADR/RID packing group	II
IMDG packing group	II
ICAO packing group	II
ADN packing group	II

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant
No.

14.6. Special precautions for user

Always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

EmS	F-A, S-G
ADR transport category	2
Emergency Action Code	1Z
Hazard Identification Number (ADR/RID)	40
Tunnel restriction code	(E)

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not applicable.

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulations	Health and Safety at Work etc. Act 1974 (as amended). The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"]. EH40/2005 Workplace exposure limits.
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TBTU (o-Benzotriazol-1-yl-N,N,N',N'-tetramethyluronium tetrafluoroborate)

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

Inventories

EU - EINECS/ELINCS

None of the ingredients are listed or exempt.

SECTION 16: Other information

Abbreviations and acronyms used in the safety data sheet	<p>ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.</p> <p>ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.</p> <p>RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.</p> <p>IATA: International Air Transport Association.</p> <p>ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air.</p> <p>IMDG: International Maritime Dangerous Goods.</p> <p>CAS: Chemical Abstracts Service.</p> <p>ATE: Acute Toxicity Estimate.</p> <p>LC50: Lethal Concentration to 50 % of a test population.</p> <p>LD50: Lethal Dose to 50% of a test population (Median Lethal Dose).</p> <p>EC₅₀: 50% of maximal Effective Concentration.</p> <p>PBT: Persistent, Bioaccumulative and Toxic substance.</p> <p>vPvB: Very Persistent and Very Bioaccumulative.</p>
Classification abbreviations and acronyms	<p>Flam. Sol. = Flammable solid</p> <p>Acute Tox. = Acute toxicity</p> <p>Eye Irrit. = Eye irritation</p> <p>Skin Irrit. = Skin irritation</p> <p>STOT SE = Specific target organ toxicity-single exposure</p>
Classification procedures according to SI 2019 No. 720	<p>Acute Tox. 4 - H302: STOT SE 3 - H335: Skin Irrit. 2 - H315: Eye Irrit. 2 - H319: : Expert judgement. Flam. Sol. 1 - H228: : Expert judgement.</p>
Training advice	<p>Only trained personnel should use this material.</p>
Revision date	<p>05/10/2022</p>
Revision	<p>1</p>
SDS number	<p>1617</p>
Hazard statements in full	<p>H228 Flammable solid.</p> <p>H302 Harmful if swallowed.</p> <p>H315 Causes skin irritation.</p> <p>H319 Causes serious eye irritation.</p> <p>H335 May cause respiratory irritation.</p>

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.