

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 06.03.2013

Version 2.5

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

1.1 Product identifier

Catalogue No.	851012
Product name	HCTU O-(1H-6-Chlorobenzotriazole-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate Novabiochem®
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

Identified uses	Peptide synthesis, Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merck-chemicals.com).
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1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number **Please contact the regional company representation in your country.**

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Flammable solid, Category 1, H228

For the full text of the H-Statements mentioned in this Section, see Section 16.

Classification (67/548/EEC or 1999/45/EC)

F Highly flammable R11

For the full text of the R-phrases mentioned in this Section, see Section 16.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H228 Flammable solid.

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hexafluorophosphate Novabiochem®

Precautionary statements

Prevention
P210 Keep away from heat.

Caution - substance not yet tested completely.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word
Danger

CAS-No. 330645-87-9

Labelling (67/548/EEC or 1999/45/EC)

Symbol(s)  F Highly flammable

R-phrases(s) 11 Highly flammable.

Further information

Caution - substance not yet tested completely.

Reduced labelling (≤125 ml)

Symbol(s)  F Highly flammable

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula C₁₁H₁₅ClF₆N₅OP (Hill)
CAS-No. 330645-87-9
Molar mass 413,69 g/mol

For the full text of the H-Statements mentioned in this Section, see Section 16.

Remarks No disclosure requirement according to Regulation (EC) No.
1907/2006

3.2 Mixture

not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air. Consult doctor if feeling unwell.

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After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water with the eyelid held wide open. Call in ophthalmologist if necessary.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

We have no description of any toxic symptoms.

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO₂), Foam, Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

Fire may cause evolution of:

Hydrogen fluoride, Hydrogen chloride gas, nitrogen oxides, Oxides of phosphorus

5.3 Advice for firefighters

Special protective equipment for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Avoid inhalation of dusts. Ensure adequate ventilation. Keep away from open flames, hot surfaces and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

6.2 Environmental precautions

Do not empty into drains.

Risk of explosion.

6.3 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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6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Dry. Tightly closed. Keep away from heat and sources of ignition.

Store at +2°C to +8°C.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

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The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

Flame retardant antistatic protective clothing

Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter P 2 (acc. to DIN 3181) for solid and liquid particles of harmful substances

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.

Environmental exposure controls

Do not empty into drains.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	solid
Colour	white
Odour	No strong odour known.
Odour Threshold	No information available.
pH	No information available.
Melting point	> 185 °C
Boiling point	No information available.
Flash point	No information available.
Evapouration rate	No information available.
Flammability (solid, gas)	The substance or mixture is a flammable solid with the category 1.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	No information available.

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Relative vapour density	No information available.
Relative density	No information available.
Water solubility	No information available.
Partition coefficient: n-octanol/water	No information available.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

Explosive

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.

10.2 Chemical stability

heat-sensitive

Sensitivity to light

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

This information is not available.

Acute inhalation toxicity

This information is not available.

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Acute dermal toxicity

This information is not available.

Skin irritation

This information is not available.

Eye irritation

This information is not available.

Sensitisation

This information is not available.

Germ cell mutagenicity

This information is not available.

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

Hazardous properties cannot be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

No information available.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Discharge into the environment must be avoided.

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SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number UN 1325
14.2 Proper shipping name FLAMMABLE SOLID, ORGANIC, N.O.S. (O-(1H-6-
CHLOROBENZOTRIAZOL--1-YL)-1,1,3,3-
TETRAMETHYLURONIUM HEXAFLUOROPHOSPHATE)
14.3 Class 4.1
14.4 Packing group II
14.5 Environmentally hazardous --
14.6 Special precautions for user yes
Tunnel restriction code E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number UN 1325
14.2 Proper shipping name FLAMMABLE SOLID, ORGANIC, N.O.S. (O-(1H-6-
CHLOROBENZOTRIAZOL--1-YL)-1,1,3,3-
TETRAMETHYLURONIUM HEXAFLUOROPHOSPHATE)
14.3 Class 4.1
14.4 Packing group II
14.5 Environmentally hazardous --
14.6 Special precautions for user no

Sea transport (IMDG)

14.1 UN number UN 1325
14.2 Proper shipping name FLAMMABLE SOLID, ORGANIC, N.O.S. (O-(1H-6-
CHLOROBENZOTRIAZOL--1-YL)-1,1,3,3-
TETRAMETHYLURONIUM HEXAFLUOROPHOSPHATE)
14.3 Class 4.1
14.4 Packing group II
14.5 Environmentally hazardous --
14.6 Special precautions for user yes
EmS F-A S-G

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

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SECTION 15. Regulatory information

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

EU regulations

Major Accident Hazard 96/82/EC
Legislation Directive 96/82/EC does not apply

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work.

National legislation

Storage class 4.1B

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

Full text of H-Statements referred to under sections 2 and 3.

H228 Flammable solid.

Full text of R-phrases referred to under sections 2 and 3

R11 Highly flammable.

Training advice

Provide adequate information, instruction and training for operators.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.