

# Voluntary safety information following the Safety Data Sheet format according to Regulation (EC) No. 1907/2006 (REACH)



**O-(1H-6-Chlorobenzotriazole-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate (HCTU) PEPTIPURE® ≥99 %**

article number: **2112**  
Version: **3.0 en**  
Replaces version of: 15.06.2022  
Version: (2)

date of compilation: 24.01.2019  
Revision: 02.03.2024

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

### 1.1 Product identifier

Identification of the substance	<b>O-(1H-6-Chlorobenzotriazole-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate (HCTU) PEPTIPURE® ≥99 %</b>
Article number	2112
Registration number (REACH)	It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a).
CAS number	330645-87-9

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for private purposes (household). Food, drink and animal feedingstuffs.

### 1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG  
Schoemperlenstr. 3-5  
D-76185 Karlsruhe  
Germany

**Telephone:**+49 (0) 721 - 56 06 0  
**Telefax:** +49 (0) 721 - 56 06 149  
**e-mail:** sicherheit@carlroth.de  
**Website:** www.carlroth.de

Competent person responsible for the safety data sheet: Department Health, Safety and Environment

**e-mail (competent person):** sicherheit@carlroth.de

### 1.4 Emergency telephone number

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

**Classification according to Regulation (EC) No 1272/2008 (CLP)**

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

### 2.2 Label elements

**Labelling according to Regulation (EC) No 1272/2008 (CLP)**

not required

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## 2.3 Other hazards

### Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

### Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	O-(1H-6-Chlorobenzotriazole-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate
Molecular formula	C <sub>11</sub> H <sub>15</sub> ClF <sub>6</sub> N <sub>5</sub> OP
Molar mass	413,7 g/mol
CAS No	330645-87-9

## SECTION 4: First aid measures

### 4.1 Description of first aid measures



#### General notes

Take off contaminated clothing.

#### Following inhalation

Provide fresh air.

#### Following skin contact

Rinse skin with water/shower.

#### Following eye contact

Rinse cautiously with water for several minutes.

#### Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

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

Symptoms and effects are not known to date.

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

none

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media



#### Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!  
water, foam, dry extinguishing powder, ABC-powder

#### Unsuitable extinguishing media

water jet

### 5.2 Special hazards arising from the substance or mixture

Combustible.

#### Hazardous combustion products

In case of fire may be liberated: Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Phosphorus oxides (P<sub>x</sub>O<sub>y</sub>)

### 5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures



#### For non-emergency personnel

Control of dust.

### 6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

### 6.3 Methods and material for containment and cleaning up

#### Advice on how to contain a spill

Covering of drains. Take up mechanically.

#### Advice on how to clean up a spill

Take up mechanically.

#### Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

### 6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

No special measures are necessary.

#### Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

### 7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place. Keep in a cool place.

#### Incompatible substances or mixtures

Observe hints for combined storage.

#### Consideration of other advice:

#### Ventilation requirements

Use local and general ventilation.

#### Specific designs for storage rooms or vessels

Recommended storage temperature: 2 – 8 °C

### 7.3 Specific end use(s)

No information available.

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### National limit values

#### Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

### 8.2 Exposure controls

#### Individual protection measures (personal protective equipment)

#### Eye/face protection



Use safety goggle with side protection.

#### Skin protection



#### • hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374.

#### • type of material

NBR (Nitrile rubber)

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- **material thickness**

>0,11 mm

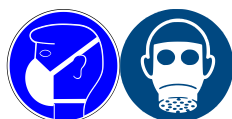
- **breakthrough times of the glove material**

>480 minutes (permeation: level 6)

- **other protection measures**

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

### Respiratory protection



Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P1 (filters at least 80 % of airborne particles, colour code: White).

### Environmental exposure controls

Keep away from drains, surface and ground water.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Physical state	solid
Colour	white
Odour	characteristic
Melting point/freezing point	>185 °C
Boiling point or initial boiling point and boiling range	not determined
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	not applicable
Auto-ignition temperature	not determined
Decomposition temperature	not relevant
pH (value)	not applicable
Kinematic viscosity	not relevant
<u>Solubility(ies)</u>	
Water solubility	not determined
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	this information is not available

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Vapour pressure	not determined
<u>Density and/or relative density</u>	
Density	not determined
Relative vapour density	Information on this property is not available.
Particle characteristics	No data available.
<u>Other safety parameters</u>	
Oxidising properties	none

## 9.2 Other information

Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
Other safety characteristics:	There is no additional information.

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

### 10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

### 10.3 Possibility of hazardous reactions

**Violent reaction with:** strong oxidiser

### 10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

### 10.5 Incompatible materials

There is no additional information.

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

## SECTION 11: Toxicological information

### 11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Classification according to GHS (1272/2008/EC, CLP)

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

#### Acute toxicity

Shall not be classified as acutely toxic.

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**Skin corrosion/irritation**

Shall not be classified as corrosive/irritant to skin.

**Serious eye damage/eye irritation**

Shall not be classified as seriously damaging to the eye or eye irritant.

**Respiratory or skin sensitisation**

Shall not be classified as a respiratory or skin sensitiser.

**Germ cell mutagenicity**

Shall not be classified as germ cell mutagenic.

**Carcinogenicity**

Shall not be classified as carcinogenic.

**Reproductive toxicity**

Shall not be classified as a reproductive toxicant.

**Specific target organ toxicity - single exposure**

Shall not be classified as a specific target organ toxicant (single exposure).

**Specific target organ toxicity - repeated exposure**

Shall not be classified as a specific target organ toxicant (repeated exposure).

**Aspiration hazard**

Shall not be classified as presenting an aspiration hazard.

**Symptoms related to the physical, chemical and toxicological characteristics**

• **If swallowed**

Data are not available.

• **If in eyes**

slightly irritant but not relevant for classification

• **If inhaled**

slightly irritant but not relevant for classification

• **If on skin**

Data are not available.

• **Other information**

This information is based upon the present state of our knowledge. Substance not yet fully tested.

**11.2 Endocrine disrupting properties**

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

**11.3 Information on other hazards**

There is no additional information.

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## SECTION 12: Ecological information

### 12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

### 12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 0,8895 mg/mg

Theoretical Oxygen Demand (with nitrification): 1,199 mg/mg

Theoretical Carbon Dioxide: 1,17 mg/mg

### 12.3 Bioaccumulative potential

Data are not available.

### 12.4 Mobility in soil

Data are not available.

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.

### 12.7 Other adverse effects

Data are not available.

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods



Consult the appropriate local waste disposal expert about waste disposal.

#### Sewage disposal-relevant information

Do not empty into drains.

#### Waste treatment of containers/packagings

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

### 13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

### 13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.



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## SECTION 14: Transport information

- 14.1 UN number or ID number** not subject to transport regulations
- 14.2 UN proper shipping name** not assigned
- 14.3 Transport hazard class(es)** none
- 14.4 Packing group** not assigned
- 14.5 Environmental hazards** non-environmentally hazardous acc. to the dangerous goods regulations
- 14.6 Special precautions for user**  
There is no additional information.
- 14.7 Maritime transport in bulk according to IMO instruments**  
The cargo is not intended to be carried in bulk.
- 14.8 Information for each of the UN Model Regulations**
- International Maritime Dangerous Goods Code (IMDG) - Additional information**  
Not subject to IMDG.
- International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information**  
Not subject to ICAO-IATA.

## SECTION 15: Regulatory information

- 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**
- Relevant provisions of the European Union (EU)**
- Restrictions according to REACH, Annex XVII**  
not listed
- List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list**  
Not listed.
- Seveso Directive**

### 2012/18/EU (Seveso III)

No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements	Notes
	not assigned		

### Deco-Paint Directive

VOC content	0 %
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### Industrial Emissions Directive (IED)

VOC content	0 %
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## Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

## Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

## Water Framework Directive (WFD)

List of pollutants (WFD)				
Name of substance	Name acc. to inventory	CAS No	Listed in	Remarks
O-(1H-6-Chlorobenzotriazole-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate	Organohalogen compounds and substances which may form such compounds in the aquatic environment		a)	
O-(1H-6-Chlorobenzotriazole-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate	Organophosphorous compounds		a)	

### Legend

a) Indicative list of the main pollutants

## Regulation on the marketing and use of explosives precursors

not listed

## Regulation on drug precursors

not listed

## Regulation on substances that deplete the ozone layer (ODS)

not listed

## Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

## Regulation on persistent organic pollutants (POP)

not listed

## Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

## National inventories

Country	Inventory	Status
TW	TCSI	substance is listed

### Legend

TCSI Taiwan Chemical Substance Inventory

## 15.2 Chemical safety assessment

No Chemical Safety Assessment has been carried out for this substance.

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## SECTION 16: Other information

### Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
14.8	Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information: Not subject to ADR, RID and ADN.		yes

### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)
ED	Endocrine disruptor
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SVHC	Substance of Very High Concern
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

### Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures. Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

### Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.