acc. to Regulation (EC) No. 1907/2006 (REACH)

1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexafluorophosphate (HDMA) PEPTIPURE® ≥98 %

article number: 6888 Version: 2.0 en Replaces version of: 2021-09-22 Version: (1)

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

Product identifier 1.1

Identification of the substance

Article number

CAS number

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

Relevant identified uses:

| Uses advised | against: |
|--------------|----------|
|--------------|----------|

Do not use for private purposes (household).

1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexafluorophosphate (HDMA) PEPTIPURE® ≥98

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 Department Health, Safety and Environment sheet:

e-mail (competent person):

1.4 **Emergency telephone number**

| Name | Street | Postal code/city | Telephone | Website |
|--|-----------|----------------------|--------------|---------|
| National Poisons Information Service City Hospital | Dudley Rd | B187QH Birmingham | 844 892 0111 | |

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS



date of compilation: 2021-09-22

Revision: 2024-03-02

958029-37-3

6888

%

Laboratory chemical Laboratory and analytical use

sicherheit@carlroth.de

Food, drink and animal feedingstuffs.

acc. to Regulation (EC) No. 1907/2006 (REACH)



1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexafluorophosphate (HDMA) PEPTIPURE® ≥98 %

article number: 6888

| Section | ction Hazard class | | Hazard class and category | Hazard statement |
|----------------------------|---|---|---------------------------|---------------------|
| 3.10 Acute toxicity (oral) | | 4 | Acute Tox. 4 | H302 |
| 3.1D | Acute toxicity (dermal) | 4 | Acute Tox. 4 | H312 |
| 3.1I | 3.1I Acute toxicity (inhal.) | | Acute Tox. 4 | H332 |
| 3.2 | 3.2 Skin corrosion/irritation | | Skin Irrit. 2 | H315 |
| 3.3 | 3.3 Serious eye damage/eye irritation | | Eye Irrit. 2 | H319 |
| 3.8R | 3.8R Specific target organ toxicity - single exposure (respirat- ory tract irritation) | | STOT SE 3 | H335 |

For full text of abbreviations: see SECTION 16

2.2 Label elements

Labelling

Signal word Warning

Pictograms

GHS07



Hazard statements

| H302+H312+H332 | Harmful if swallowed, in contact with skin or if inhaled |
|----------------|--|
| H315 | Causes skin irritation |
| H319 | Causes serious eye irritation |
| H335 | May cause respiratory irritation |

Precautionary statements

Precautionary statements - prevention

| P261 | Avoid breathing dust |
|------|---------------------------------------|
| P280 | Wear protective gloves/eye protection |

Precautionary statements - response

| P302+P352 | IF ON SKIN: Wash with plenty of water |
|----------------|---|
| 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

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 $\ge 0,1\%$.

acc. to Regulation (EC) No. 1907/2006 (REACH)



1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexa-

fluorophosphate (HDMA)

1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexafluorophosphate (HDMA) PEPTIPURE® ≥98 %

article number: 6888

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance

Molecular formula $C_{12}H_{17}F_6N_6O_2P$ Molar mass $422,3^{g}/_{mol}$ CAS No958029-37-3

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

Following ingestion

Rinse mouth with water (only if the person is conscious). Call a doctor.

4.2 Most important symptoms and effects, both acute and delayed

Vomiting, Irritation, Cough, Dyspnoea

4.3 Indication of any immediate medical attention and special treatment needed none

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

acc. to Regulation (EC) No. 1907/2006 (REACH)

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article number: 6888

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 (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂), Phosphorus oxides (PxOy), Hydrogen fluoride (HF)

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

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. Do not breathe 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. Control of dust.

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.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation. Avoid dust formation.

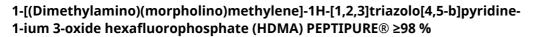
Measures to prevent fire as well as aerosol and dust generation

Removal of dust deposits.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

acc. to Regulation (EC) No. 1907/2006 (REACH)



article number: 6888

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

Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted. 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)

| Coun try | Name of agent | CAS No | Identifi- er | TWA [mg/ m³] | STEL [mg/ m³] | Ceil- ing-C [mg/ m³] | Nota- tion | Source |
|-------------|---------------|--------|-----------------|--------------------|---------------------|-------------------------------|---------------|-----------|
| GB | dust | | WEL | 10 | | | i | EH40/2005 |
| GB | dust | | WEL | 4 | | | r | EH40/2005 |

Notation

 Ceiling-C
 Ceiling value is a limit value above which exposure should not occur

 i
 Inhalable fraction

 r
 Respirable fraction

 STEL
 Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15minute period (unless otherwise specified)

 TWA
 Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection





acc. to Regulation (EC) No. 1907/2006 (REACH)



1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexafluorophosphate (HDMA) PEPTIPURE® ≥98 %

article number: 6888

hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a consider-able reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

• type of material

NBR (Nitrile rubber)

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). P2 (filters at least 94 % 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 |
|--|---|
| Form | powder, crystalline |
| Colour | whitish |
| Odour | characteristic |
| Melting point/freezing point | 218 °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 |

acc. to Regulation (EC) No. 1907/2006 (REACH)

article number: 6888

1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexafluorophosphate (HDMA) PEPTIPURE® ≥98 %



| Decomposition temperature | not relevant |
|---|--|
| pH (value) | not applicable |
| Kinematic viscosity | not relevant |
| Colubility/ioc) | |
| Solubility(ies) | |
| Water solubility | not determined |
| Partition coefficient | |
| Partition coefficient n-octanol/water (log value): | this information is not available |
| | |
| Vapour pressure | not determined |
| | |
| Density and/or relative density | |
| Density | not determined |
| Relative vapour density | Information on this property is not available. |
| | |
| Particle characteristics | No data available. |
| Other setety never store | |
| Other safety parameters | |
| Oxidising properties | none |
| 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

9.2

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.

acc. to Regulation (EC) No. 1907/2006 (REACH)



1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexafluorophosphate (HDMA) PEPTIPURE® ≥98 %

article number: 6888

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Harmful if swallowed. Harmful in contact with skin. Harmful if inhaled.

Skin corrosion/irritation

Causes skin irritation.

Serious eye damage/eye irritation

Causes serious eye irritation.

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

May cause respiratory irritation.

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

Causes serious eye irritation

If inhaled

Irritation to respiratory tract, cough, Dyspnoea

• If on skin

causes skin irritation

Other information

none

11.2 Endocrine disrupting properties

acc. to Regulation (EC) No. 1907/2006 (REACH)

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1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexafluorophosphate (HDMA) PEPTIPURE® ≥98 %

article number: 6888

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

11.3 Information on other hazards

There is no additional information.

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): 0,9092 $^{mg}/_{mg}$ Theoretical Oxygen Demand (with nitrification): 1,266 $^{mg}/_{mg}$ Theoretical Carbon Dioxide: 1,251 $^{mg}/_{mg}$

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 $\ge 0,1\%$.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

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.

Properties of waste which render it hazardous

- **HP 4** irritant skin irritation and eye damage
- HP 5 specific target organ toxicity (STOT)/aspiration toxicity
- **HP6** acute toxicity

acc. to Regulation (EC) No. 1907/2006 (REACH)



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article number: 6888

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.

SECTION 14: Transport information

14.1 UN number or ID number

- 14.2 UN proper shipping name
- 14.3 Transport hazard class(es)
- 14.4 Packing group
- 14.5 Environmental hazards

not subject to transport regulations

not assigned

none

not assigned

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)

Seveso Directive

| 2012/18/EU (Seveso III) | | | | | |
|--|--------------|---|--|--|--|
| No Dangerous substance/hazard categories | | Qualifying quantity (tonnes) for the application of lower and upper-tier requirements | | | |
| | not assigned | | | | |

Deco-Paint Directive

| VOC content | 0 % |
|-------------|-----|
|-------------|-----|

Industrial Emissions Directive (IED)

VOC content

0 %

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

acc. to Regulation (EC) No. 1907/2006 (REACH)



1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexafluorophosphate (HDMA) PEPTIPURE® ≥98 %

article number: 6888

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 | |
| 1- [(Dimethylamino)(morpholino)me thylene]-1H-[1,2,3]triazolo[4,5- b]pyridine-1-ium 3-oxide hexa- fluorophosphate (HDMA) | Organohalogen compounds and substances which may form such compounds in the aquatic envir- onment | | a) | | |
| 1- [(Dimethylamino)(morpholino)me thylene]-1H-[1,2,3]triazolo[4,5- b]pyridine-1-ium 3-oxide hexa- fluorophosphate (HDMA) | 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

National regulations(GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list not listed

Restrictions according to GB REACH, Annex 17

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.

15.2 Chemical safety assessment

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

acc. to Regulation (EC) No. 1907/2006 (REACH)



1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexafluorophosphate (HDMA) PEPTIPURE® ≥98 %

article number: 6888

SECTION 16: Other information

Indication of changes (revised safety data sheet)

| Section | Former entry (text/value) | Actual entry (text/value) | Safety- relev- ant |
|---------|--|---|--------------------------|
| 2.2 | Labelling of packages where the contents do not exceed 125 ml: Signal word: Warning | | yes |
| 2.2 | | Labelling of packages where the contents do not exceed 125 ml: change in the listing (table) | yes |
| 2.2 | | Labelling of packages where the contents do not exceed 125 ml: change in the listing (table) | yes |
| 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 in- formation: Not subject to ADR, RID and ADN. | | yes |
| 15.1 | Restrictions according to REACH, Annex XVII | | yes |
| 15.1 | | Dangerous substances with restrictions (REACH, Annex XVII): change in the listing (table) | yes |
| 15.1 | List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list: Not listed. | | yes |
| 15.1 | | National regulations(GB) | yes |
| 15.1 | | List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list: not listed | yes |
| 15.1 | | Restrictions according to GB REACH, Annex 17: not listed | yes |

Abbreviations and acronyms

| Abbr. | Descriptions of used abbreviations |
|-----------|--|
| ADR | Accord relatif au transport international des marchandises dangereuses par route (Agreement concern- ing the International Carriage of Dangerous Goods by Road) |
| CAS | Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances) |
| Ceiling-C | Ceiling value |
| DGR | Dangerous Goods Regulations (see IATA/DGR) |
| ED | Endocrine disruptor |
| EH40/2005 | EH40/2005 Workplace exposure limits (http://www.nationalarchives.gov.uk/doc/open-government-li- cence/) |
| GB REACH | The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended) |
| GHS | "Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Na- tions |

acc. to Regulation (EC) No. 1907/2006 (REACH)



1-[(Dimethylamino)(morpholino)methylene]-1H-[1,2,3]triazolo[4,5-b]pyridine-1-ium 3-oxide hexafluorophosphate (HDMA) PEPTIPURE® ≥98 %

article number: 6888

| Abbr. | Descriptions of used abbreviations |
|----------|--|
| ΙΑΤΑ | 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 |
| РВТ | Persistent, Bioaccumulative and Toxic |
| REACH | Registration, Evaluation, Authorisation and Restriction of Chemicals |
| RID | Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regula- tions concerning the International carriage of Dangerous goods by Rail) |
| STEL | Short-term exposure limit |
| TWA | Time-weighted average |
| VOC | Volatile Organic Compounds |
| vPvB | Very Persistent and very Bioaccumulative |
| WEL | Workplace exposure limit |

Key literature references and sources for data

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

List of relevant phrases (code and full text as stated in section 2 and 3)

| Code | Text |
|------|-----------------------------------|
| H302 | Harmful if swallowed. |
| H312 | Harmful in contact with skin. |
| H315 | Causes skin irritation. |
| H319 | Causes serious eye irritation. |
| H332 | Harmful if inhaled. |
| H335 | May cause respiratory irritation. |

Disclaimer

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