



according to Regulation (EC) No 1907/2006

PyBOP

Revision date: 17.08.2021 Product code: RL-2005 Page 1 of 12

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

1.1. Product identifier

PyBOP

Further trade names

Benzotriazol-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphat Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate (Benzotriazol-1-yloxy)tripyrrolidinophosphonium hexafluorophosphate

PYBOP hexafluorophosphate

Phosphorus(1+), [1-(hydroxy-O)-1H-benzotriazolato]tri-1-pyrrolidinyl-, (T-4)-, hexafluorophosphate(1-) (1:1) Substance name: Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate

(PyBOP)

REACH Registration Number: 01-2120823727-49-XXXX

128625-52-5 CAS No: EC No: 60-329-0

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

Use of the substance/mixture

Manufacture of the substance. Laboratory chemical

Uses advised against

Do not use for private purposes (household). Restrictions on use: Pharmaceutical substance

1.3. Details of the supplier of the safety data sheet

Company name: Iris Biotech GmbH

Street: Adalbert-Zoellner-Straße 1 Place: D-95615 Marktredwitz, Germany

Post-office box:

D-95605 Marktredwitz, Germany

Telephone: Telefax: +49 9231 97121 99 +49 9231 97121 0

e-mail: info@iris-biotech.de

Contact person: Compliance Department Telephone: +49 9231 97121 0

sds@iris-biotech.de e-mail: Internet: www.iris-biotech.de

Responsible Department: Only available during office hours.

+49 (0)89 19240 (POISON CENTER Munich: 24 h) 1.4. Emergency telephone

number:

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Acute Tox. 4; H302 Skin Sens. 1; H317 Aquatic Acute 1: H400 Aquatic Chronic 1; H410

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Warning



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Pictograms:





Hazard statements

H302 Harmful if swallowed.

H317 May cause an allergic skin reaction.

H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P272 Contaminated work clothing should not be allowed out of the workplace.

P273 Avoid release to the environment.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing

protection.

P301+P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.

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

P333+P313 If skin irritation or rash occurs: Get medical advice/attention.
P501 Dispose of contents/container to an approved disposal site.

Additional advice on labelling

Warning - substance not yet tested completely.

2.3. Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1. Substances

Chemical characterization

Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate

Sum formula: C18H28N6OP*PF6
Molecular weight: 375,43*144,96 g/mol

Hazardous components

CAS No	Chemical name			Quantity	
	EC No	Index No	REACH No		
	Classification (Regulation (EC) No 1272/2008)				
128625-52-5	Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate (PyBOP)			100 %	
	60-329-0		01-2120823727-49-XXXX		
	Acute Tox. 4, Skin Sens. 1, Aquatic Acute 1, Aquatic Chronic 1; H302 H317 H400 H410				

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
	Specific Conc. Limits, M-factors and ATE		
128625-52-5	60-329-0	Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate (PyBOP)	100 %
inhalation: Data lacking (gases); dermal: Data lacking; oral: LD50 = <300 - >2000 mg/kg			

SECTION 4: First aid measures

4.1. Description of first aid measures





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General information

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

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

After inhalation

Provide fresh air. Remove casualty to fresh air and keep warm and at rest. In case of irregular breathing or respiratory arrest provide artificial respiration.

After contact with skin

Wash with plenty of water. Take off contaminated clothing and wash it before reuse. After contact with skin, wash immediately with plenty of water and soap.

After contact with eyes

Rinse immediately carefully and thoroughly with eye-bath or water. In case of eye irritation consult an ophthalmologist. In case of contact with eyes, rinse immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart. Subsequently consult an ophthalmologist.

After ingestion

Medical treatment necessary. Rinse mouth thoroughly with water. Never give anything by mouth to an unconscious person or a person with cramps.

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

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

Refer to chapter 11.

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

Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings. Water spray. alcohol resistant foam. Dry extinguishing powder. Carbon dioxide (CO2). Sand.

Unsuitable extinguishing media

High power water jet.

5.2. Special hazards arising from the substance or mixture

Non-flammable. Thermal decomposition can lead to the escape of irritating gases and vapours.

In case of fire may be liberated: Carbon dioxide (CO2). Carbon monoxide (CO). Nitrogen oxides (NOx).

Phosphorus oxides. Fluorhydric acid.

5.3. Advice for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing. Full protection suit.

Additional information

Suppress gases/vapours/mists with water spray jet. Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water. Usual measures for fire prevention.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General advice

Provide adequate ventilation. Avoid breathing dust/fume/gas/mist/vapours/spray.

Avoid contact with skin, eyes and clothes.

Wear personal protection equipment.

In case of fire: Evacuate area.

For non-emergency personnel

Take up carefully when dry.





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For emergency responders

Take up mechanically, placing in appropriate containers for disposal. Take up dust-free and set down dust-free

6.2. Environmental precautions

Do not allow to enter into soil/subsoil.

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up

For cleaning up

Take up mechanically. Treat the recovered material as prescribed in the section on waste disposal.

Other information

Take up mechanically, placing in appropriate containers for disposal. Avoid dust formation.

Clear contaminated areas thoroughly.

6.4. Reference to other sections

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13 Treat the recovered material as prescribed in the section on waste disposal.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

If handled uncovered, arrangements with local exhaust ventilation have to be used. Avoid dust formation. Do not breathe dust. Provide adequate ventilation.

Avoid dust formation. Avoid breathing dust/fume/gas/mist/vapours/spray.

Avoid contact with skin, eyes and clothes.

Advice on protection against fire and explosion

Usual measures for fire prevention.

Advice on general occupational hygiene

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme.

Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat, drink, smoke, sniff. Avoid contact with skin, eyes and clothes.

Provide adequate ventilation. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container tightly closed. Keep container tightly closed in a cool, well-ventilated place.

Handle and store contents under inert gas. Protect from moisture.

Protect from sunlight. Sensitivity to light.

May cause decomposition by long-term light influence.

storage temperature: +2°C - +8°C

Hints on joint storage

No special measures are necessary.

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

Additional advice on limit values

Contains no substances with occupational exposure limit values.

8.2. Exposure controls





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Appropriate engineering controls

The receiver of our product is singularly responsible for adhering to existing laws and regulations.

Individual protection measures, such as personal protective equipment

Eye/face protection

Wear eye/face protection.

Tightly fitting safety goggles. Face shield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Hand protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. 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. Wear suitable gloves.

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Skin protection

Use of protective clothing.

Respiratory protection

In case of inadequate ventilation wear respiratory protection. If technical exhaust or ventilation measures are not possible or insufficient, respiratory protection must be worn.

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Environmental exposure controls

Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state: solid

Colour: white/ whitish
Odour: No data available
Odour threshold: not determined

Test method

Changes in the physical state

Melting point/freezing point: 150 (decomposition) °C OECD 102

Boiling point or initial boiling point and not applicable

boiling range:

Sublimation point: not determined Softening point: not determined





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Flash point: not applicable

Flammability

Solid/liquid: not applicable
Gas: not applicable

Explosive properties

The product is not: Explosive.

Lower explosion limits:

Upper explosion limits:

not determined

not determined

Auto-ignition temperature:

not determined

Self-ignition temperature

Solid: not applicable
Gas: not applicable
Decomposition temperature: 150 °C
pH-Value: not determined
Viscosity / dynamic: not applicable
Viscosity / kinematic: not applicable
Flow time: not applicable

Water solubility: 0,7182 g/L OECD 105

(at 20 °C)

Solubility in other solvents

No data available

Dissolution rate: not determined

Partition coefficient n-octanol/water: Log Kow (Log Pow): -0.3 (26 °C) OECD 107

Dispersion stability: not determined Vapour pressure: not applicable

Density (at 20 °C): 1,438 g/cm³ OECD 109

Bulk density:

Relative vapour density:

not determined

9.2. Other information

Information with regard to physical hazard classes

Sustaining combustion: No data available

Oxidizing properties

UN Test O.1: Test for oxidising solids Not oxidising.

GHS/CLP criteria are not met.

Other safety characteristics

Solid content: not determined Evaporation rate: not determined

Further Information

SECTION 10: Stability and reactivity

10.1. Reactivity

Product is not dust explosive in its original delivery form. The addition of particulate matter, however, results in a dust explosion risk.

10.2. Chemical stability

Stable under recommended storage conditions.



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10.3. Possibility of hazardous reactions

No data available

10.4. Conditions to avoid

Protect from moisture. Moisture-sensitive.

Keep away from heat.

Protect from direct sunlight. Sensitivity to light.

10.5. Incompatible materials

Violent reaction with: Oxidizing agents, strong.

10.6. Hazardous decomposition products

Thermal decomposition can lead to the escape of irritating gases and vapours.

In case of fire may be liberated: Carbon dioxide (CO2). Carbon monoxide (CO). Nitrogen oxides (NOx).

Fluorhydric acid. Phosphorus oxides.

Further information

In case of fire: See chapter 5.

SECTION 11: Toxicological information

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

Toxicocinetics, metabolism and distribution

No data available

Acute toxicity

Harmful if swallowed.

CAS No	Chemical name					
	Exposure route	Dose	Species	Source	Method	
128625-52-5	Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate (PyBOP)					
	oral	LD50 <300 - >2000 mg/kg	Rat	ECHA	OECD 423	
	dermal	Data lacking				
	inhalation	Data lacking				

Irritation and corrosivity

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

Skin corrosion/irritation:

Skin - EPISKIN Human Skin Model Test

Result: No skin irritation

OECD 439

Serious eye damage/eye irritation:

eyes: In vitro eye test Result: No eye irritation

OECD 492

Sensitising effects

May cause an allergic skin reaction. (Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate (PyBOP))

Respiratory or skin sensitisation:

In Chemico Skin Sensitisation: Direct Peptide Reactivity Assay (DPRA)

Result: positive.
OECD 442C
In-vitro-Test:
Result: positive.

OECD 442D



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Carcinogenic/mutagenic/toxic effects for reproduction

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

Germ cell mutagenicity:

Ames test

Escherichia coli/ Salmonella typhimurium

OECD 471 (Ames test)

STOT-single exposure

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

STOT-repeated exposure

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

Aspiration hazard

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

Specific effects in experiment on an animal

No data available

Additional information on tests

No data available

Practical experience

No data available

11.2. Information on other hazards

Endocrine disrupting properties

No data available

Other information

No data available

Further information

This substance is classified as hazardous according to Regulation (EC) No 1272 (2008).

RTECS: No data available

Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia.

Caution! To the best of our knowledge the toxicological properties of this material have not been thoroughly investigated. Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1. Toxicity

Very toxic to aquatic life with long lasting effects.

CAS No	Chemical name						
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method	
128625-52-5	Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate (PyBOP)						
	Acute algae toxicity	ErC50 2,54 mg/l		Pseudokirchneriella subcapitata	ECHA	OECD 201	
	Acute crustacea toxicity	EC50 0,25 mg/l		Daphnia magna (Big water flea)	ECHA	OECD 202	

12.2. Persistence and degradability



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CAS No	Chemical name				
	Method	Value	d	Source	
	Evaluation				
128625-52-5	Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate (PyBOP)				
	Biodegradability: aerobic.	0 %	28	OECD 301F	
	Not readily biodegradable (according to OECD criteria)		•		

12.3. Bioaccumulative potential

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
128625-52-5	Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate (PyBOP)	-0,3

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

No data available

12.7. Other adverse effects

Warning - substance not yet tested completely.

Further information

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal recommendations

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil. Dispose of waste according to applicable legislation. Dispose of waste according to applicable legislation.

Consult the appropriate local waste disposal expert about waste disposal.

Contaminated packaging

Non-contaminated packages may be recycled. Handle contaminated packages in the same way as the substance itself. Handle contaminated packages in the same way as the substance itself.

SECTION 14: Transport information

Land transport (ADR/RID)

UN 3077 14.1. UN number or ID number:

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. 14.2. UN proper shipping name:

(Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate

(PyBOP))

14.3. Transport hazard class(es):

14.4. Packing group: Hazard label:

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Classification code:



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Special Provisions: 274 335 375 601

Limited quantity: 5 kg
Excepted quantity: E1
Transport category: 3
Hazard No: 90
Tunnel restriction code: -

Inland waterways transport (ADN)

14.1. UN number or ID number: UN 3077

14.2. UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.

(Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate

(PyBOP))

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14.3. Transport hazard class(es):

14.4. Packing group: Hazard label:

Classification code: M7

Special Provisions: 274 335 375 601

Limited quantity: 5 kg
Excepted quantity: E1

Marine transport (IMDG)

14.1. UN number or ID number: UN 3077

14.2. UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.

(Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate

(PyBOP))

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14.3. Transport hazard class(es):

14.4. Packing group:

Hazard label:



Special Provisions: 274, 335, 966, 967, 969

Limited quantity: 5 kg
Excepted quantity: E1
EmS: F-A, S-F

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number: UN 3077

14.2. UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.

 $(Benzotriazole\hbox{-}1\hbox{-}yl\hbox{-}oxy\hbox{-}tris\hbox{-}pyrrolidino\hbox{-}phosphonium\ hexafluorophosphate}$

(PyBOP))

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14.3. Transport hazard class(es):

14.4. Packing group:
Hazard label:

Special Provisions: A97 A158 A179 A197 A215

Limited quantity Passenger: 30 kg G
Passenger LQ: Y956
Excepted quantity: E1

IATA-packing instructions - Passenger:

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IATA-max. quantity - Passenger:400 kgIATA-packing instructions - Cargo:956IATA-max. quantity - Cargo:400 kg

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: Yes



Danger releasing substance: Benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate

(PyBOP)

14.6. Special precautions for user

No data available

14.7. Maritime transport in bulk according to IMO instruments

not applicable

Other applicable information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids

SECTION 15: Regulatory information

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

EU regulatory information

Information according to 2012/18/EU

E1 Hazardous to the Aquatic Environment

(SEVESO III):

Additional information

Safety Data Sheet according to Regulation (EC) No. 1907/2006 (REACH)

National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile

work protection guideline' (94/33/EC).

Water hazard class (D): 3 - highly hazardous to water

Skin resorption/Sensitization: Causes allergic hypersensitivity reactions.

15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

SECTION 16: Other information

Abbreviations and acronyms

CLP: Classification, labelling and Packaging

REACH: Registration, Evaluation and Authorization of Chemicals

GHS: Globally Harmonised System of Classification, Labelling and Packaging of Chemicals

UN: United Nations

CAS: Chemical Abstracts Service
DNEL: Derived No Effect Level
DMEL: Derived Minimal Effect Level
PNEC: Predicted No Effect Concentration

ATE: Acute toxicity estimate LC50: Lethal concentration, 50%

LD50: Lethal dose, 50% LL50: Lethal loading, 50% EL50: Effect loading, 50%

EC50: Effective Concentration 50%

ErC50: Effective Concentration 50%, growth rate



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NOEC: No Observed Effect Concentration

BCF: Bio-concentration factor

PBT: persistent, bioaccumulative, toxic vPvB: very persistent, very bioaccumulative

ADR: Accord européen sur le transport des marchandises dangereuses par Route

(European Agreement concerning the International Carriage of Dangerous Goods by Road)

RID: Regulations concerning the international carriage of dangerous goods by rail

ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways (Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures)

IMDG: International Maritime Code for Dangerous Goods

EmS: Emergency Schedules MFAG: Medical First Aid Guide

IATA: International Air Transport Association ICAO: International Civil Aviation Organization

MARPOL: International Convention for the Prevention of Marine Pollution from Ships

IBC: Intermediate Bulk Container SVHC: Substance of Very High Concern

For abbreviations and acronyms, see table at http://abbrev.esdscom.eu

Relevant H and EUH statements (number and full text)

H302 Harmful if swallowed.

H317 May cause an allergic skin reaction.

H400 Very toxic to aquatic life.

H410 Very toxic to aquatic life with long lasting effects.

Further Information

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights. The receiver of our product is singularly responsible for adhering to existing laws and regulations. Warning - substance not yet tested completely.

The product is intended for research, analysis and scientific education.

The receiver of our product is singularly responsible for adhering to existing laws and regulations.

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights.

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.