

**Safety Data Sheet**

according to UK REACH Regulation

**4-Pentynoyl-Val-Ala-PAB-PNP**

Revision date: 20.10.2023

Product code: ADC1320

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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1. Product identifier**

4-Pentynoyl-Val-Ala-PAB-PNP

**Further trade names**

4-Pentynoyl-va-PAB-PNP, 4-((S)-2-((S)-3-methyl-2-pent-4-ynamidobutanamido)propanamido)benzyl

4-nitrophenyl carbonate, 4-pentynoyl-valyl-alanyl-(4-aminobenzyl)-(4-nitrophenyl)-carbonate

CAS No: 1956294-76-0

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

Laboratory chemical. Manufacture of the substance.

**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:	568	
	D-95605 Marktredwitz, Germany	
Telephone:	+49 9231 97121 0	Telefax: +49 9231 97121 99
E-mail:	info@iris-biotech.de	
Contact person:	Compliance Department	Telephone: +49 9231 97121 0
E-mail:	sds@iris-biotech.de	
Internet:	www.iris-biotech.de	
Responsible Department:	Only available during office hours.	

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

This product does not meet the criteria for classification into a hazardous class according to Regulation (EC) No 1272/2008 on the classification, labeling and packaging of substances and mixtures. A safety data sheet is provided which does not fully comply with Article 31 and Annex II of REACH.

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

**SECTION 2: Hazards identification****2.1. Classification of the substance or mixture****GB CLP Regulation**

This substance is not classified as hazardous in accordance with GB CLP Regulation.

**2.2. Label elements****GB CLP Regulation****Precautionary statements**

P202	Do not handle until all safety precautions have been read and understood.
P261	Avoid breathing dust/fume/gas/mist/vapours/spray.
P262	Do not get in eyes, on skin, or on clothing.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.

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**Additional advice on labelling**

Labelling according to Regulation (EC) No. 1272/2008 [CLP]: none (GHS/CLP criteria are not met.)

Warning - substance not yet tested completely.

**2.3. Other hazards**

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

**SECTION 3: Composition/information on ingredients****3.1. Substances****Chemical characterization**

4-pentynoyl-valyl-alanyl-(4-aminobenzyl)-(4-nitrophenyl)-carbonate

Sum formula: C<sub>27</sub>H<sub>30</sub>N<sub>4</sub>O<sub>8</sub>

Molecular weight: 538,55 g/mol

**Hazardous components**

none (according to UK REACH Regulation)

**SECTION 4: First aid measures****4.1. Description of first aid measures****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. If product gets into the eye, keep eyelid open and rinse immediately with large quantities of water, for at least 5 minutes. Subsequently consult an ophthalmologist.

**After ingestion**

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

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

No information available.

**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. Sand.

**Unsuitable extinguishing media**

High power water jet.

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**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 (CO<sub>2</sub>). Carbon monoxide (CO). Nitrogen oxides (NO<sub>x</sub>).

**5.3. Advice for firefighters**

In case of fire: Wear self-contained breathing apparatus.

**Additional information**

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**

Remove all sources of ignition. Provide adequate ventilation.  
Use personal protection equipment.

**For emergency responders**

Wear personal protection equipment (refer to section 8).  
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 containment**

Avoid dust formation.

**For cleaning up**

Take up mechanically.

**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**

Provide adequate ventilation.  
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**

Take off contaminated clothing. Wash hands before breaks and after work. When using do not eat, drink,

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smoke, sniff. Avoid contact with skin, eyes and clothes. Provide adequate ventilation.

**7.2. Conditions for safe storage, including any incompatibilities****Requirements for storage rooms and vessels**

Keep container tightly closed in a cool, well-ventilated place.  
Handle and store contents under inert gas. Protect from moisture.  
storage temperature: -20°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**

To date, no national critical limit values exist.

**8.2. Exposure controls****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).

**Thermal hazards**

No data available

**Environmental exposure controls**

Discharge into the environment must be avoided.

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**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:	No data available	
Melting point/freezing point:		No data available
Boiling point or initial boiling point and boiling range:		No data available
Flammability:		not determined
Lower explosion limits:		No data available
Upper explosion limits:		No data available
Flash point:		No data available
Auto-ignition temperature:		No data available
Decomposition temperature:		No data available
pH-Value:		No data available
Viscosity / kinematic:		not applicable
Water solubility:		No data available
Solubility in other solvents		
not determined		
Dissolution rate:		No data available
Partition coefficient n-octanol/water:		No data available
Dispersion stability:		No data available
Vapour pressure:		No data available
Density:		No data available
Relative density:		No data available
Bulk density:		No data available
Relative vapour density:		No data available
Particle characteristics:		No data available

**9.2. Other information****Information with regard to physical hazard classes**

## Explosive properties

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

Sustaining combustion: No data available

## Self-ignition temperature

Solid: No data available

Gas: not applicable

## Oxidizing properties

No data available

**Other safety characteristics**

Solvent content: No data available

Viscosity / dynamic: not applicable

Flow time: not applicable

**SECTION 10: Stability and reactivity****10.1. Reactivity**

No data available

**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.

Keep away from heat.

**10.5. Incompatible materials**

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 (CO<sub>2</sub>). Carbon monoxide (CO). Nitrogen oxides (NO<sub>x</sub>).**Further information**

In case of fire: See chapter 5.

**SECTION 11: Toxicological information****11.1. Information on hazard classes as defined in GB CLP Regulation****Toxicokinetics, metabolism and distribution**

No data available

**Acute toxicity**

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

**Irritation and corrosivity**

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

**Sensitising effects**

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

**Carcinogenic/mutagenic/toxic effects for reproduction**

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

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

**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.

**Information on likely routes of exposure**

No data available

**Specific effects in experiment on an animal**

No data available

**Additional information on tests**

The substance is classified as not hazardous according to regulation (EC) No 1272/2008 [CLP].

**Practical experience**

No data available

**11.2. Information on other hazards****Endocrine disrupting properties**

No data available

**Further information**

RTECS: No data available

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.

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Handle in accordance with good industrial hygiene and safety practice.

**SECTION 12: Ecological information****12.1. Toxicity**

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

**12.2. Persistence and degradability**

No data available

**12.3. Bioaccumulative potential**

No data available

**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 UK REACH.

**12.6. Endocrine disrupting properties**

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

**12.7. Other adverse effects**

Warning - substance not yet tested completely.

**Further information**

Avoid release to the environment.

**SECTION 13: Disposal considerations****13.1. Waste treatment methods****Disposal recommendations**

Dispose of waste according to applicable legislation.

Consult the appropriate local waste disposal expert about waste disposal.

Handle contaminated packages in the same way as the substance itself.

**Contaminated packaging**

Wash with plenty of water. Completely emptied packages can be recycled.

**SECTION 14: Transport information****Land transport (ADR/RID)****14.2. UN proper shipping name:**

No dangerous good in sense of these transport regulations.

**Inland waterways transport (ADN)****14.2. UN proper shipping name:**

No dangerous good in sense of these transport regulations.

**Marine transport (IMDG)****14.2. UN proper shipping name:**

No dangerous good in sense of these transport regulations.

**Air transport (ICAO-TI/IATA-DGR)****14.2. UN proper shipping name:**

No dangerous good in sense of these transport regulations.

**14.5. Environmental hazards**

ENVIRONMENTALLY HAZARDOUS: No

**14.6. Special precautions for user**

No information available.

**14.7. Maritime transport in bulk according to IMO instruments**

not applicable

**SECTION 15: Regulatory information****15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture**

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**EU regulatory information**

Information according to 2012/18/EU (SEVESO III): Not subject to 2012/18/EU (SEVESO III)

**Additional information**

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

**National regulatory information**

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

**15.2. Chemical safety assessment**

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

**SECTION 16: Other information****Abbreviations and acronyms**

ADR: Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road).  
IMDG: International Maritime Code for Dangerous Goods  
IATA: International Air Transport Association  
GHS: Globally Harmonized System of Classification and Labelling of Chemicals  
EINECS: European Inventory of Existing Commercial Chemical Substances  
ELINCS: European List of Notified Chemical Substances  
CAS: Chemical Abstracts Service  
LC50: Lethal concentration, 50%  
LD50: Lethal dose, 50%  
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  
LL50: Lethal loading, 50%  
EL50: Effect loading, 50%  
EC50: Effective Concentration 50%  
ErC50: Effective Concentration 50%, growth rate  
NOEC: No Observed Effect Concentration  
BCF: Bio-concentration factor  
PBT: persistent, bioaccumulative, toxic  
vPvB: very persistent, very bioaccumulative  
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)  
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>



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#### 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.