

## SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 21.11.2010

Version 3.3

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

#### 1.1 Product identifier

Catalogue No.	820963
Product name	1-Pentyne for synthesis
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	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal ( <a href="http://www.merck-chemicals.com">www.merck-chemicals.com</a> ).
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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: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

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

### 2. Hazards identification

#### 2.1 Classification of the substance or mixture

**Classification (REGULATION (EC) No 1272/2008)**

Flammable liquid, Category 2, H225

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

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

F; 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*

H225 Highly flammable liquid and vapour.

*Precautionary statements*

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P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.  
P223 Keep away from any possible contact with water, because of violent reaction and possible flash fire.  
P403 + P235 Store in a well-ventilated place. Keep cool.

**Reduced labelling (≤125 ml)**

*Hazard pictograms*



*Signal word*

Danger

CAS-No. 627-19-0

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

Symbol(s)	F	Highly flammable
R-phrase(s)	11	Highly flammable.
S-phrase(s)	16-29	Keep away from sources of ignition - No smoking. Do not empty into drains.
EC-No.	210-987-1	

**Reduced labelling (≤125 ml)**

Symbol(s) F Highly flammable

**2.3 Other hazards**

None known.

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**3. Composition/information on ingredients**

Formula	C <sub>5</sub> H <sub>8</sub> (Hill)
CAS-No.	627-19-0
EC-No.	210-987-1
Molar mass	68,11 g/mol

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**4. First aid measures**

**4.1 Description of first aid measures**

After inhalation: fresh air.

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

After eye contact: rinse out with plenty of water.

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Call a physician immediately.

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

narcosis

**4.3 Indication of immediate medical attention and special treatment needed**

No information available.

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## 5. Fire-fighting measures

### 5.1 Extinguishing media

*Suitable extinguishing media*

Carbon dioxide (CO<sub>2</sub>), 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 material, Vapours are heavier than air and may spread along floors.

Pay attention to flashback.

Forms explosive mixtures with air at ambient temperatures.

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

### 5.3 Advice for firefighters

*Special protective equipment for fire-fighters*

In the event of fire, wear self-contained breathing apparatus.

*Further information*

Prevent fire extinguishing water from contaminating surface water or the ground water system.

Remove container from danger zone and cool with water.

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## 6. Accidental release measures

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

Advice for non-emergency personnel: Avoid substance contact. Do not breathe vapours, aerosols. Ensure adequate ventilation. 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 7.2 and 10.5).

Take up with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

### 6.4 Reference to other sections

Indications about waste treatment see section 13.

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## 7. Handling and storage

### 7.1 Precautions for 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.

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

Keep away from heat and sources of ignition. Keep container tightly closed in a dry and well-ventilated place.

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Store at +2°C to +8°C.

### 7.3 Specific end uses

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

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## 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.

#### *Hygiene measures*

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

#### *Eye/face protection*

Safety glasses

#### *Hand protection*

full contact:

Glove material:	Viton (R)
Glove thickness:	0,70 mm
Break through time:	> 480 min

splash contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 30 min

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 890 Vitoject® (full contact), KCL 898 Butoject® (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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](http://www.kcl.de)).

#### *Other protective equipment:*

Flame retardant antistatic protective clothing

#### *Respiratory protection*

required when vapours/aerosols are generated.

#### *Environmental exposure controls*

Do not empty into drains.

Risk of explosion.

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## 9. Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	malodorous
Odour Threshold	No information available.
pH	No information available.
Melting point	-106 °C
Boiling point/boiling range	39 - 41 °C at 1.013 hPa
Flash point	-20 °C Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	467 hPa at 20 °C
Relative vapour density	2,4
Relative density	0,69 g/cm <sup>3</sup> at 20 °C
Water solubility	1,05 g/l at 25 °C
Partition coefficient: n-octanol/water	log Pow: 1,98 Method: (experimental) (Lit.) No remarkable bioaccumulation potential is expected (log Pow 1-3).
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	No information available.

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Oxidizing properties No information available.

## 9.2 Other data

none

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## 10. Stability and reactivity

### 10.1 Reactivity

Vapours may form explosive mixture with air.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapours with:

Violent reactions possible with:

Oxidizing agents

Risk of explosion with:

perchlorates, silver

### 10.4 Conditions to avoid

Warming.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### 10.5 Incompatible materials

no information available

### 10.6 Hazardous decomposition products

no information available

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## 11. Toxicological information

### 11.1 Information on toxicological effects

#### *Acute oral toxicity*

Symptoms: Risk of aspiration upon vomiting., Aspiration may cause pulmonary oedema and pneumonitis.

#### *Specific target organ toxicity - single exposure*

The substance or mixture is not classified as specific target organ toxicant, single exposure.

#### *Specific target organ toxicity - repeated exposure*

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

#### *Aspiration hazard*

No aspiration toxicity classification

### 11.2 Further information

#### *Further information*

Quantitative data on the toxicity of this product are not available.

Further toxicological data:

Property that cannot be excluded on the basis of structure- effect considerations:

After uptake of large quantities:

narcosis

Further data:

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Other dangerous properties can not be excluded.  
Handle in accordance with good industrial hygiene and safety practice.

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## 12. Ecological information

### 12.1 Toxicity

No information available.

### 12.2 Persistence and degradability

No information available.

### 12.3 Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: 1,98

Method: (experimental)

(Lit.) No remarkable bioaccumulation potential is expected (log Pow 1-3).

### 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

*Additional ecological information*

We have no quantitative data concerning the ecological effects of this product.

Further information on ecology

Do not allow to run into surface waters, wastewater, or soil.

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## 13. Disposal considerations

*Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## 14. Transport information

### ADR/RID

UN 1993 FLAMMABLE LIQUID, N.O.S. (1-PENTYNE), 3, II

### IATA

UN 1993 FLAMMABLE LIQUID, N.O.S. (1-PENTYNE), 3, II

### IMDG

UN 1993 FLAMMABLE LIQUID, N.O.S. (1-PENTYNE), 3, II

EmS F-E S-E

The transport regulations are cited according to international regulations and in the form applicable in Germany. Possible national deviations in other countries are not considered.

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## 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	Highly flammable
	7b
	Quantity 1: 5.000 t
	Quantity 2: 50.000 t

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

*National legislation*

Storage class VCI 3 Flammable Liquids

**15.2 Chemical Safety Assessment**

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

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**16. Other information**

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

H225 Highly flammable liquid and vapour.

**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.

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

**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](http://www.wikipedia.org).

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*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.*