

## SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 17.04.2013

Version 4.0

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

#### 1.1 Product identifier

Catalogue No. 807061  
Product name 1,5-Pentanediol for synthesis  
REACH Registration Number 01-2119449341-44-XXXX

#### 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 ([www.merck-chemicals.com](http://www.merck-chemicals.com)).

#### 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: [prodsafe@merckgroup.com](mailto:prodsafe@merckgroup.com)

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

### SECTION 2. Hazards identification

#### 2.1 Classification of the substance or mixture

This substance is not classified as dangerous according to European Union legislation.

#### 2.2 Label elements

##### Labelling (REGULATION (EC) No 1272/2008)

Not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008.

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

The product does not need to be labelled in accordance with EC directives or respective national laws.

#### 2.3 Other hazards

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

### SECTION 3. Composition/information on ingredients

#### 3.1 Substance

Formula  $C_5H_{12}O_2$  (Hill)  
CAS-No. 111-29-5  
EC-No. 203-854-4  
Molar mass 104,15 g/mol

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

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 807061  
Product name 1,5-Pentanediol for synthesis

---

Remarks No disclosure requirement according to Regulation (EC) No. 1907/2006

**3.2 Mixture**  
not applicable

---

**SECTION 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: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

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

Drowsiness, Dizziness, Unconsciousness, inebriation

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

No information available.

---

**SECTION 5. Firefighting 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.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

**5.3 Advice for firefighters**

*Special protective equipment for firefighters*

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.

---

**SECTION 6. Accidental release measures**

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

Advice for non-emergency personnel: Do not breathe vapours, aerosols. 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.

**6.3 Methods and materials for containment and cleaning up**

---

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 807061  
Product name 1,5-Pentanediol for synthesis

---

Cover drains. Collect, bind, and pump off spills.  
Observe possible material restrictions (see sections 7 and 10).  
Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

#### 6.4 Reference to other sections

Indications about waste treatment see section 13.

---

### SECTION 7. Handling and storage

#### 7.1 Precautions for safe handling

*Advice on safe handling*

Observe label precautions.

*Hygiene measures*

Change contaminated clothing. Wash hands after working with substance.

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

*Storage conditions*

Tightly closed.

Store at +15°C to +25°C.

#### 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

##### Derived No Effect Level (DNEL)

Worker DNEL, longterm	Systemic effects	inhalation	59 mg/m <sup>3</sup>
Worker DNEL, longterm	Systemic effects	dermal	17 mg/kg Body weight
Consumer DNEL, acute	Systemic effects	oral	25 mg/kg Body weight
Consumer DNEL, longterm	Systemic effects	inhalation	14,5 mg/m <sup>3</sup>
Consumer DNEL, longterm	Systemic effects	dermal	8,5 mg/kg Body weight
Consumer DNEL, longterm	Systemic effects	oral	4,3 mg/kg Body weight

##### Predicted No Effect Concentration (PNEC)

PNEC Fresh water	0,5 mg/l
PNEC Fresh water sediment	1,05 mg/kg
PNEC Marine water	0,05 mg/l
PNEC Marine sediment	0,105 mg/kg
PNEC Aquatic intermittent release	5 mg/l
PNEC Sewage treatment plant	170,7 mg/l
PNEC Soil	0,0764 mg/kg

#### 8.2 Exposure controls

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 807061  
Product name 1,5-Pentanediol for synthesis

---

**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.

*Eye/face protection*

Safety glasses

*Hand protection*

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 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 741 Dermatril® L (full contact), KCL 741 Dermatril® L (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)).

*Respiratory protection*

Not required; except in case of aerosol formation.

**Environmental exposure controls**

Do not empty into drains.

---

**SECTION 9. Physical and chemical properties**

**9.1 Information on basic physical and chemical properties**

Form	liquid
Colour	colourless
Odour	odourless
Odour Threshold	not applicable
pH	7,5
Melting point	-16 °C

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 807061  
Product name 1,5-Pentanediol for synthesis

---

Boiling point/boiling range	240 - 242 °C at 1.013 hPa
Flash point	136 °C
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1,3 %(V)
Upper explosion limit	13,1 %(V)
Vapour pressure	> 0,01 hPa at 20 °C
Relative vapour density	No information available.
Relative density	0,99 g/cm <sup>3</sup> at 20 °C
Water solubility	at 20 °C soluble
Partition coefficient: n-octanol/water	log Pow: -0,49 (experimental) (External MSDS) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	500 °C
Viscosity, dynamic	110 mPa.s at 20 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

## 9.2 Other data

Ignition temperature	330 °C
----------------------	--------

---

## SECTION 10. Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, strong reducing agents, acid halides, Acid anhydrides

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 807061  
Product name 1,5-Pentanediol for synthesis

---

**10.4 Conditions to avoid**

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

**10.5 Incompatible materials**

no information available

**10.6 Hazardous decomposition products**

no information available

---

**SECTION 11. Toxicological information**

**11.1 Information on toxicological effects**

*Acute oral toxicity*

LD50 rat: 10.000 mg/kg (External MSDS)

*Acute inhalation toxicity*

This information is not available.

*Acute dermal toxicity*

LD50 rabbit: > 19.800 mg/kg (IUCLID)

*Skin irritation*

rabbit

Result: No irritation

(External MSDS)

*Eye irritation*

rabbit

Result: No eye irritation

(External MSDS)

*Sensitisation*

This information is not available.

*Germ cell mutagenicity*

*Genotoxicity in vitro*

Ames test

Result: negative

Method: OECD Test Guideline 471

*Carcinogenicity*

This information is not available.

*Reproductive toxicity*

This information is not available.

*Teratogenicity*

This information is not available.

*Specific target organ toxicity - single exposure*

This information is not available.

*Specific target organ toxicity - repeated exposure*

This information is not available.

*Aspiration hazard*

This information is not available.

**11.2 Further information**

After absorption of large quantities:

---

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 807061  
Product name 1,5-Pentanediol for synthesis

---

Systemic effects:

Dizziness, Drowsiness, inebriation, Unconsciousness

No toxic effects are to be expected when the product is handled appropriately.

Handle in accordance with good industrial hygiene and safety practice.

---

**SECTION 12. Ecological information**

**12.1 Toxicity**

*Toxicity to fish*

LC50 Leuciscus idus (Golden orfe): 4.600 mg/l; 96 h (External MSDS)

*Toxicity to daphnia and other aquatic invertebrates*

EC50 Daphnia magna (Water flea): > 500 mg/l; 48 h (External MSDS)

*Toxicity to algae*

IC50 Desmodesmus subspicatus (green algae): > 500 mg/l; 72 h (External MSDS)

*Toxicity to bacteria*

EC50 Pseudomonas putida: 230 mg/l; 17 h (External MSDS)

**12.2 Persistence and degradability**

*Biodegradability*

99 %; 14 d

OECD Test Guideline 302B

Readily eliminated from water

**12.3 Bioaccumulative potential**

*Partition coefficient: n-octanol/water*

log Pow: -0,49

(experimental)

(External MSDS) Bioaccumulation is not expected.

**12.4 Mobility in soil**

No information available.

**12.5 Results of PBT and vPvB assessment**

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

**12.6 Other adverse effects**

*Additional ecological information*

When discharged properly, no impairments in the function of adapted biological wastewater treatment plants are to be expected.

Discharge into the environment must be avoided.

---

**SECTION 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.

---

**SECTION 14. Transport information**

**Land transport (ADR/RID)**

14.1 - 14.6

Not classified as dangerous in the meaning of transport regulations.

**Inland waterway transport (ADN)**

Not relevant

**Air transport (IATA)**

---

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 807061  
Product name 1,5-Pentanediol for synthesis

---

**14.1 - 14.6** Not classified as dangerous in the meaning of transport regulations.

**Sea transport (IMDG)**

**14.1 - 14.6** Not classified as dangerous in the meaning of transport regulations.

**14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code**

Not relevant

---

**SECTION 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 Directive 96/82/EC does not apply

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Regulation (EC) No 689/2008 concerning the export and import of dangerous chemicals not regulated

Substances of very high concern (SVHC) This product does not contain substances of very high concern above the respective regulatory limit (> 0.1 % (w/w) Regulation (EC) No 1907/2006 (REACH), Article 57).

*National legislation*

Storage class 10

**15.2 Chemical Safety Assessment**

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

---

**SECTION 16. Other information**

**Training advice**

Provide adequate information, instruction and training for operators.

**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).

**Regional representation**

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

---

*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.*

---