

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



1-Pentanol ~98%, for synthesis

article number: **8949**
Version: **1.0 en**

date of compilation: 2017-03-01

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

1.1 Product identifier

| | |
|---------------------------------|------------------------------------|
| Identification of the substance | 1-Pentanol |
| Article number | 8949 |
| Registration number (REACH) | This information is not available. |
| Index No | 603-200-00-1 |
| EC number | 200-752-1 |
| CAS number | 71-41-0 |

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

Identified uses: laboratory chemical

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

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Telefax: +49 (0) 721 - 56 06 149

e-mail: sicherheit@carlroth.de

Website: www.carlroth.de

Competent person responsible for the safety data sheet : Department Health, Safety and Environment

e-mail (competent person) : sicherheit@carlroth.de

1.4 Emergency telephone number

Emergency information service **Poison Centre Munich: +49/(0)89 19240**

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

| Classification acc. to GHS | | | |
|----------------------------|---|---------------------------|------------------|
| Section | Hazard class | Hazard class and category | Hazard statement |
| 2.6 | flammable liquid | (Flam. Liq. 3) | H226 |
| 3.1I | acute toxicity (inhal.) | (Acute Tox. 4) | H332 |
| 3.2 | skin corrosion/irritation | (Skin Irrit. 2) | H315 |
| 3.8R | specific target organ toxicity - single exposure (respiratory tract irritation) | (STOT SE 3) | H335 |

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2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP)

Signal word

Warning

Pictograms



Hazard statements

| | |
|------|----------------------------------|
| H226 | Flammable liquid and vapour |
| H315 | Causes skin irritation |
| H332 | Harmful if inhaled |
| H335 | May cause respiratory irritation |

Precautionary statements

Precautionary statements - prevention

| | |
|------|---|
| P210 | Keep away from heat, hot surfaces, sparks, open flames. No smoking. |
| P260 | Do not breathe mist/vapours. |

Precautionary statements - response

| | |
|-----------|---|
| P302+P352 | IF ON SKIN: Wash with plenty of soap and water. |
| P312 | Call a POISON CENTER/doctor if you feel unwell. |

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Warning**

Symbol(s)



2.3 Other hazards

There is no additional information.

SECTION 3: Composition/information on ingredients

3.1 Substances

| | |
|-------------------|----------------------------------|
| Name of substance | n-Amyl alcohol |
| Index No | 603-200-00-1 |
| EC number | 200-752-1 |
| CAS number | 71-41-0 |
| Molecular formula | C ₅ H ₁₂ O |
| Molar mass | 88,15 g/mol |

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SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. If breathing is irregular or stopped, administer artificial respiration. Medical treatment necessary.

Following skin contact

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

Following eye contact

Rinse cautiously with water for several minutes. In case of eye irritation consult an ophthalmologist.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Irritation, Cough, Headache, Vertigo, Nausea, Vomiting, Diarrhoea, Dyspnoea, Unconsciousness

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 fire-fighting measures to the fire surroundings
water spray, foam, alcohol resistant foam, dry extinguishing powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours can form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: carbon monoxide (CO), carbon dioxide (CO₂)

5.3 Advice for firefighters

Vapours are heavier than air. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

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SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Do not breathe vapour/spray. Avoid contact with skin and eyes. Avoidance of ignition sources.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Explosive properties.

6.3 Methods and material for containment and cleaning up

Advices on how to contain a spill

Covering of drains.

Advices on how to clean up a spill

Absorb with liquid-binding material (e.g. sand, diatomaceous earth, acid- or universal binding agents).

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

Avoid: Aerosol or mist formation. Provide adequate ventilation. When not in use, keep containers tightly closed.

• Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge.

Advice on general occupational hygiene

Wash hands before breaks and after work.

7.2 Conditions for safe storage, including any incompatibilities

Store in a well-ventilated place. Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice

Ground/bond container and receiving equipment.

• Ventilation requirements

Use local and general ventilation.

• Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C.

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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)

Data are not available.

Relevant DNELs/DMELs/PNECs and other threshold levels

• human health values

| Endpoint | Threshold level | Protection goal, route of exposure | Used in | Exposure time |
|----------|-------------------------|------------------------------------|-------------------|-------------------------|
| DNEL | 73,16 mg/m ³ | human, inhalatory | worker (industry) | chronic - local effects |
| DNEL | 292 mg/m ³ | human, inhalatory | worker (industry) | acute - local effects |

• environmental values

| Endpoint | Threshold level | Environmental compartment |
|----------|-----------------|------------------------------|
| PNEC | 0,12 mg/l | freshwater |
| PNEC | 0,012 mg/l | marine water |
| PNEC | 1,2 mg/l | water |
| PNEC | 37 mg/l | sewage treatment plant (STP) |
| PNEC | 0,496 mg/kg | freshwater sediment |
| PNEC | 0,05 mg/kg | marine sediment |
| PNEC | 1,068 mg/kg | soil |

8.2 Exposure controls

Individual protection measures (personal protective equipment)



Eye/face protection

Use safety goggles with side protection.

Skin protection

• 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.

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- **type of material**

NBR (Nitrile rubber)

- **material thickness**

0,4 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: Aerosol or mist formation. Type: ABEK (combined filters against gases and vapours, colour code: Brown/Grey/Yellow/Green).

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

Appearance

| | |
|-----------------|-------------------|
| Physical state | liquid (fluid) |
| Colour | colourless |
| Odour | characteristic |
| Odour threshold | No data available |

Other physical and chemical parameters

| | |
|---|--|
| pH (value) | 7 (22 g/l, 20 °C) |
| Melting point/freezing point | -78 °C |
| Initial boiling point and boiling range | 138 °C |
| Flash point | 47 °C |
| Evaporation rate | no data available |
| Flammability (solid, gas) | not relevant (fluid) |
| <u>Explosive limits</u> | |
| • lower explosion limit (LEL) | 1,6 vol% |
| • upper explosion limit (UEL) | 8 vol% |
| Explosion limits of dust clouds | not relevant |
| Vapour pressure | 2,6 hPa at 20 °C |
| Density | 0,81 - 0,83 g/cm ³ at 20 °C |
| Vapour density | 3,04 (air = 1) |
| Bulk density | Not applicable |
| Relative density | Information on this property is not available. |

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Solubility(ies)

Water solubility 22 g/l at 20 °C

Partition coefficient

n-octanol/water (log KOW) 1,51 (exp. Lit.)

Auto-ignition temperature 300 °C

Decomposition temperature 450 °C

Viscosity not determined

Explosive properties Shall not be classified as explosive

Oxidising properties none

9.2 Other information

Refractive index 1,409 - 1,412

Temperature class (EU, acc. to ATEX) T2 (Maximum permissible surface temperature on the equipment: 300°C)

SECTION 10: Stability and reactivity

10.1 Reactivity

Risk of ignition. In case of warming: Vapours can form explosive mixtures with air.

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: Oxygen, Strong oxidiser, Alkali metals, Aldehydes, Alkaline earth metal, Acids, Hydrogen, Sulphuric acid, Chlorine,
=> Explosive properties

10.4 Conditions to avoid

Keep away from heat. Decomposition takes place from temperatures above: 450 °C.

10.5 Incompatible materials

Rubber articles, different plastics

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

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SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

| Exposure route | Endpoint | Value | Species | Source |
|----------------|----------|--------------|---------|--------|
| oral | LD50 | >2.000 mg/kg | rat | |
| dermal | LD50 | >2.000 mg/kg | rabbit | |

Skin corrosion/irritation

Causes skin irritation.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor 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**

diarrhoea, vomiting, nausea, Liver and kidney damage

- **If in eyes**

Irritating to eyes

- **If inhaled**

cough, Irritation to respiratory tract, breathing difficulties

- **If on skin**

has degreasing effect on the skin, causes skin irritation

Other information

Other adverse effects: Headache, Vertigo, Dyspnoea, Unconsciousness

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SECTION 12: Ecological information

12.1 Toxicity

acc. to 1272/2008/EC: Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)

| Endpoint | Value | Species | Source | Exposure time |
|----------|----------|--------------------------|--------|---------------|
| EC50 | 341 mg/l | daphnia magna | IUCLID | 48 h |
| LC50 | 530 mg/l | zebra fish (Danio rerio) | | 96 h |

12.2 Process of degradability

The substance is readily biodegradable.
Theoretical Oxygen Demand: 2,722 mg/mg
Theoretical Carbon Dioxide: 2,496 mg/mg
Biochemical Oxygen Demand: 1,25 g/g

| Process | Degradation rate | Time |
|----------------|------------------|------|
| biotic/abiotic | 80 - 90 % | 28 d |

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW) 1,51

12.4 Mobility in soil

Data are not available.

Henry's law constant 1,34 Pa m³/mol at 25 °C

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 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

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

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.

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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.

SECTION 14: Transport information

| | | |
|------|---|--|
| 14.1 | UN number | 1105 |
| 14.2 | UN proper shipping name | PENTANOLS |
| | Hazardous ingredients | 1-Pentanol |
| 14.3 | Transport hazard class(es) | |
| | Class | 3 (flammable liquids) |
| 14.4 | Packing group | III (substance presenting low danger) |
| 14.5 | Environmental hazards | none (non-environmentally hazardous acc. to the dangerous goods regulations) |
| 14.6 | Special precautions for user | |
| | Provisions for dangerous goods (ADR) should be complied within the premises. | |
| 14.7 | Transport in bulk according to Annex II of MARPOL and the IBC Code | |
| | The cargo is not intended to be carried in bulk. | |
| 14.8 | Information for each of the UN Model Regulations | |
| | • Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) | |
| | UN number | 1105 |
| | Proper shipping name | PENTANOLS |
| | Particulars in the transport document | UN1105, PENTANOLS, 3, III, (D/E) |
| | Class | 3 |
| | Classification code | F1 |
| | Packing group | III |
| | Danger label(s) | 3 |
| |  | |
| | Excepted quantities (EQ) | E1 |
| | Limited quantities (LQ) | 5 L |
| | Transport category (TC) | 3 |
| | Tunnel restriction code (TRC) | D/E |
| | Hazard identification No | 30 |
| | Emergency Action Code | 3YE |

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• International Maritime Dangerous Goods Code (IMDG)

| | |
|--|--------------------------------------|
| UN number | 1105 |
| Proper shipping name | PENTANOLS |
| Particulars in the shipper's declaration | UN1105, PENTANOLS, 3, III, 47°C c.c. |
| Class | 3 |
| Packing group | III |
| Danger label(s) | 3 |



| | |
|--------------------------|----------|
| Special provisions (SP) | 223 |
| Excepted quantities (EQ) | E1 |
| Limited quantities (LQ) | 5 L |
| EmS | F-E, S-D |
| Stowage category | A |

• International Civil Aviation Organization (ICAO-IATA/DGR)

| | |
|--|--------------------------|
| UN number | 1105 |
| Proper shipping name | Pentanol |
| Particulars in the shipper's declaration | UN1105, Pentanol, 3, III |
| Class | 3 |
| Packing group | III |
| Danger label(s) | 3 |



| | |
|--------------------------|------|
| Special provisions (SP) | A3 |
| Excepted quantities (EQ) | E1 |
| Limited quantities (LQ) | 10 L |

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)

- Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)
Not listed.

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15.2 Chemical Safety Assessment

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

SECTION 16: Other information

Abbreviations and acronyms

| Abbr. | Descriptions of used abbreviations |
|----------|---|
| ADN | Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways) |
| ADR | Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road) |
| CAS | Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances) |
| CLP | Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures |
| CMR | Carcinogenic, Mutagenic or toxic for Reproduction |
| DGR | Dangerous Goods Regulations (see IATA/DGR) |
| DMEL | Derived Minimal Effect Level |
| DNEL | Derived No-Effect Level |
| EINECS | European Inventory of Existing Commercial Chemical Substances |
| ELINCS | European List of Notified Chemical Substances |
| EmS | Emergency Schedule |
| GHS | "Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations |
| IATA | 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 |
| index No | the Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008 |
| MARPOL | International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant") |
| NLP | No-Longer Polymer |
| PBT | Persistent, Bioaccumulative and Toxic |
| PNEC | Predicted No-Effect Concentration |
| REACH | Registration, Evaluation, Authorisation and Restriction of Chemicals |
| RID | Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail) |
| VOC | Volatile Organic Compounds |
| vPvB | very Persistent and very Bioaccumulative |

Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)
- Dangerous Goods Regulations (DGR) for the air transport (IATA)
- International Maritime Dangerous Goods Code (IMDG)

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

| Code | Text |
|------|----------------------------------|
| H226 | flammable liquid and vapour |
| H315 | causes skin irritation |
| H332 | harmful if inhaled |
| H335 | may cause respiratory irritation |

Disclaimer

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.