

# 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: 01.03.2017

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

### 1.1 Product identifier

Identification of the substance	<b>1-Pentanol</b>
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

**Telephone:** +49 (0) 721 - 56 06 0

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

**e-mail:** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

**Website:** [www.carlroth.de](http://www.carlroth.de)

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

**e-mail (competent person)** : [sicherheit@carlroth.de](mailto: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
3.11	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 <sub>5</sub> H <sub>12</sub> 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 (CO<sub>2</sub>)

##### 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 (CO<sub>2</sub>)

#### 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 <sup>3</sup>	human, inhalatory	worker (industry)	chronic - local effects
DNEL	292 mg/m <sup>3</sup>	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 <sup>3</sup> 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 m<sup>3</sup>/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

#### • 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

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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 Pentanols

Particulars in the shipper's declaration UN1105, Pentanols, 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.

- **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**

Not listed.

- **Regulation 850/2004/EC on persistent organic pollutants (POP)**

Not listed.

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### • Restrictions according to REACH, Annex XVII

Name of substance	Wt%	Type of registration	No
1-Pentanol	100	1907/2006/EC annex XVII	3
1-Pentanol	100	1907/2006/EC annex XVII	40

### • List of substances subject to authorisation (REACH, Annex XIV)

not listed

### • Seveso Directive

#### 2012/18/EU (Seveso III)

No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements	Notes
P5c	flammable liquids (cat. 2, 3)	5.000 50.000	51)

#### Notation

51) Flammable liquids, categories 2 or 3 not covered by P5a and P5b

### • Limitation of emissions of volatile organic compounds due to the use of organic solvents in certain paints and varnishes and vehicle refinishing products (2004/42/EC, Deco-Paint Directive)

VOC content 100 %

### • Directive on industrial emissions (VOCs, 2010/75/EU)

VOC content 100 %

### Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II

not listed

### Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

### Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

not listed

### National inventories

Substance is listed in the following national inventories:

- EINECS/ELINCS/NLP (Europe)
- DSL/NDSL (Canada)
- REACH (Europe)
- Toxic Substance Control Act (TSCA)

## 15.2 Chemical Safety Assessment

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

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### 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.