

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



1,5-Pentanediol ≥98 % for synthesis

article number: **23X2**
Version: **2.0 en**
Replaces version of: 14.09.2023
Version: (1)

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Revision: 02.03.2024

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

1.1 Product identifier

| | |
|---------------------------------|---|
| Identification of the substance | 1,5-Pentanediol ≥98 % for synthesis |
| Article number | 23X2 |
| Registration number (REACH) | It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a). |
| EC number | 203-854-4 |
| CAS number | 111-29-5 |

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

| | |
|---------------------------|---|
| Relevant identified uses: | Laboratory and analytical use Laboratory chemical |
| Uses advised against: | Do not use for private purposes (household). Food, drink and animal feedingstuffs. |

1.3 Details of the supplier of the safety data sheet

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

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

2.2 Label elements

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

not required

2.3 Other hazards

Special danger of slipping by leaking/spilling product.

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Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

SECTION 3: Composition/information on ingredients

3.1 Substances

| | |
|-------------------|-----------------|
| Name of substance | 1,5-Pentanediol |
| Molecular formula | $C_5H_{12}O_2$ |
| Molar mass | 104,1 g/mol |
| CAS No | 111-29-5 |
| EC No | 203-854-4 |

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In all cases of doubt, or when symptoms persist, seek medical advice.

Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Symptoms and effects are not known to date.

4.3 Indication of any immediate medical attention and special treatment needed

none

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SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!
water spray, alcohol resistant foam, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

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

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

No special measures are necessary.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains.

Other information relating to spills and releases

Place in appropriate containers for disposal.

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.

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed. Hygroscopic.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C

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)

This information is not available.

Human health values

| Relevant DNELs and other threshold levels | | | | |
|---|----------------------|------------------------------------|-------------------|----------------------------|
| Endpoint | Threshold level | Protection goal, route of exposure | Used in | Exposure time |
| DNEL | 35 mg/m ³ | human, inhalatory | worker (industry) | chronic - systemic effects |
| DNEL | 10 mg/kg bw/day | human, dermal | worker (industry) | chronic - systemic effects |

Environmental values

| Relevant PNECs and other threshold levels | | | | |
|---|-----------------|-------------------|------------------------------|------------------------------|
| End-point | Threshold level | Organism | Environmental compartment | Exposure time |
| PNEC | 170,7 mg/l | aquatic organisms | sewage treatment plant (STP) | short-term (single instance) |

8.2 Exposure controls

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Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



- **hand protection**

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374.

- **type of material**

NBR (Nitrile rubber)

- **material thickness**

>0,11 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: A (against organic gases and vapours with a boiling point of > 65 °C , colour code: Brown).

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

| | |
|--|------------------------------|
| Physical state | liquid |
| Form | viscous |
| Colour | clear - colourless |
| Odour | odourless |
| Melting point/freezing point | -16 °C |
| Boiling point or initial boiling point and boiling range | 237,9 °C at 1.013 hPa (ECHA) |

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| | |
|---------------------------------|---|
| Flammability | this material is combustible, but will not ignite readily |
| Lower and upper explosion limit | not determined |
| Flash point | 142 °C at 1.013 hPa (ECHA) |
| Auto-ignition temperature | 330 °C at 1.013 hPa (ECHA) |
| Decomposition temperature | 500 °C |
| pH (value) | not determined |
| Kinematic viscosity | not determined |
| Dynamic viscosity | 135 mPa s at 20 °C |

Solubility(ies)

Water solubility miscible in any proportion

Partition coefficient

Partition coefficient n-octanol/water (log value): -0,49 (25 °C) (ECHA)

Vapour pressure not determined

Density and/or relative density

Density 0,985 g/cm³ at 25,2 °C (ECHA)

Relative vapour density Information on this property is not available.

Particle characteristics not relevant (liquid)

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard classes: hazard classes acc. to GHS (physical hazards): not relevant

Other safety characteristics:

Miscibility completely miscible with water

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

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SECTION 10: Stability and reactivity

10.1 Reactivity

This material is not reactive under normal ambient conditions.

If heated

Vapours may 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: strong oxidiser

10.4 Conditions to avoid

Keep away from heat. Decomposition takes place from temperatures above: 500 °C. Protect from moisture.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

Classification according to GHS (1272/2008/EC, CLP)

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

Acute toxicity

Shall not be classified as acutely toxic.

| Acute toxicity | | | | | |
|----------------|----------|---------------|---------|--------|--------|
| Exposure route | Endpoint | Value | Species | Method | Source |
| oral | LD50 | 10.000 mg/kg | rat | | ECHA |
| dermal | LD50 | >19.800 mg/kg | rabbit | | ECHA |

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

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.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

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Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

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**

Data are not available.

• **If in eyes**

Data are not available.

• **If inhaled**

Data are not available.

• **If on skin**

Data are not available.

• **Other information**

Health effects are not known.

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

| Aquatic toxicity (acute) | | | | |
|--------------------------|------------|-----------------------|--------|---------------|
| Endpoint | Value | Species | Source | Exposure time |
| LC50 | 4.640 mg/l | fish | ECHA | 96 h |
| EC50 | >500 mg/l | aquatic invertebrates | ECHA | 48 h |

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| Aquatic toxicity (chronic) | | | | |
|----------------------------|------------|----------------|--------|---------------|
| Endpoint | Value | Species | Source | Exposure time |
| EC50 | 234,5 mg/l | microorganisms | ECHA | 17 h |

12.2 Persistence and degradability

Theoretical Oxygen Demand: 2,151 mg/mg
Theoretical Carbon Dioxide: 2,113 mg/mg

Biodegradation

The substance is readily biodegradable.

| Process of degradability | | |
|--------------------------|------------------|------|
| Process | Degradation rate | Time |
| DOC removal | 98 % | 28 d |
| oxygen depletion | 95 % | 28 d |

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

| | |
|---------------------------|----------------------|
| n-octanol/water (log KOW) | -0,49 (25 °C) (ECHA) |
|---------------------------|----------------------|

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



Consult the appropriate local waste disposal expert about waste disposal.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packages

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

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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.

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. Non-contaminated packages may be recycled.

SECTION 14: Transport information

- 14.1 UN number or ID number** not subject to transport regulations
- 14.2 UN proper shipping name** not assigned
- 14.3 Transport hazard class(es)** none
- 14.4 Packing group** not assigned
- 14.5 Environmental hazards** non-environmentally hazardous acc. to the dangerous goods regulations
- 14.6 Special precautions for user**
There is no additional information.
- 14.7 Maritime transport in bulk according to IMO instruments**
The cargo is not intended to be carried in bulk.
- 14.8 Information for each of the UN Model Regulations**
 - International Maritime Dangerous Goods Code (IMDG) - Additional information**
Not subject to IMDG.
 - International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information**
Not subject to ICAO-IATA.

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)

Restrictions according to REACH, Annex XVII

not listed

List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list

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 |
| | not assigned | | |

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Deco-Paint Directive

| | |
|-------------|-------|
| VOC content | 100 % |
|-------------|-------|

Industrial Emissions Directive (IED)

| | |
|-------------|-------|
| VOC content | 100 % |
|-------------|-------|

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

not listed

Regulation on the marketing and use of explosives precursors

not listed

Regulation on drug precursors

not listed

Regulation on substances that deplete the ozone layer (ODS)

not listed

Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

Regulation on persistent organic pollutants (POP)

not listed

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

| Country | Inventory | Status |
|---------|------------|---------------------|
| AU | AIIC | substance is listed |
| CA | DSL | substance is listed |
| CN | IECSC | substance is listed |
| EU | ECSI | substance is listed |
| EU | REACH Reg. | substance is listed |
| JP | CSCL-ENCS | substance is listed |
| KR | KECI | substance is listed |
| MX | INSQ | substance is listed |
| NZ | NZIoC | substance is listed |
| PH | PICCS | substance is listed |

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| Country | Inventory | Status |
|---------|-----------|------------------------------|
| TW | TCSI | substance is listed |
| VN | NCI | substance is listed |
| US | TSCA | substance is listed (ACTIVE) |

Legend

| | |
|------------|---|
| AIIC | Australian Inventory of Industrial Chemicals |
| CSCL-ENCS | List of Existing and New Chemical Substances (CSCL-ENCS) |
| DSL | Domestic Substances List (DSL) |
| ECSI | EC Substance Inventory (EINECS, ELINCS, NLP) |
| IECSC | Inventory of Existing Chemical Substances Produced or Imported in China |
| INSQ | National Inventory of Chemical Substances |
| KECI | Korea Existing Chemicals Inventory |
| NCI | National Chemical Inventory |
| NZIoC | New Zealand Inventory of Chemicals |
| PICCS | Philippine Inventory of Chemicals and Chemical Substances (PICCS) |
| REACH Reg. | REACH registered substances |
| TCSI | Taiwan Chemical Substance Inventory |
| TSCA | Toxic Substance Control Act |

15.2 Chemical safety assessment

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

SECTION 16: Other information

Indication of changes (revised safety data sheet)

| Section | Former entry (text/value) | Actual entry (text/value) | Safety-relevant |
|---------|---|--|-----------------|
| 2.3 | Endocrine disrupting properties: Does not contain an endocrine disruptor (EDC) in a concentration of ≥ 0,1%. | Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%. | yes |

Abbreviations and acronyms

| Abbr. | Descriptions of used abbreviations |
|--------|---|
| ADR | Accord relatif au transport international des marchandises dangereuses par route (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 |
| DGR | Dangerous Goods Regulations (see IATA/DGR) |
| DNEL | Derived No-Effect Level |
| EC50 | Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval |
| EC No | The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union) |
| ED | Endocrine disruptor |
| EINECS | European Inventory of Existing Commercial Chemical Substances |
| ELINCS | European List of Notified Chemical Substances |
| GHS | "Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations |

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| Abbr. | Descriptions of used abbreviations |
|----------|---|
| 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 |
| LC50 | Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval |
| LD50 | Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval |
| NLP | No-Longer Polymer |
| PBT | Persistent, Bioaccumulative and Toxic |
| PNEC | Predicted No-Effect Concentration |
| REACH | Registration, Evaluation, Authorisation and Restriction of Chemicals |
| SVHC | Substance of Very High Concern |
| VOC | Volatile Organic Compounds |
| vPvB | Very Persistent and very Bioaccumulative |

Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures. Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.