

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



1,6-Hexanediol $\geq 96\%$, for synthesis

article number: **1CP5**
Version: **3.0 en**
Replaces version of: 2022-04-14
Version: (2)

date of compilation: 2020-07-21
Revision: 2024-03-01

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

1.1 Product identifier

Identification of the substance	1,6-Hexanediol $\geq 96\%$, for synthesis
Article number	1CP5
Registration number (REACH)	01-2119449814-31-xxxx
EC number	211-074-0
CAS number	629-11-8

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
Germany

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

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Centre Beaumont Hospital	Beaumont Road	Dublin 9	+353 1 809 2166	https://www.poisons.ie/

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

1,6-Hexanediol ≥ 96 %, for synthesis

article number: **1CP5**

2.3 Other hazards

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	1,6-Hexanediol
Molecular formula	$C_6H_{14}O_2$
Molar mass	118,2 g/mol
REACH Reg. No	01-2119449814-31-xxxx
CAS No	629-11-8
EC No	211-074-0

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

Irritant effects

4.3 Indication of any immediate medical attention and special treatment needed

none

1,6-Hexanediol ≥ 96 %, for synthesis

article number: 1CP5

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!
water, foam, alcohol resistant foam, dry extinguishing powder, ABC-powder

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. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically.

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.

1,6-Hexanediol ≥ 96 %, for synthesis

article number: 1CP5

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

Store in a dry place.

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	0,5 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0,05 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	8.400 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	1,05 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,105 mg/kg	aquatic organisms	marine sediment	short-term (single instance)

1,6-Hexanediol ≥ 96 %, for synthesis

article number: 1CP5

Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0,076 ^{mg} /kg	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

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**

>0,3 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: Dust formation. Particulate filter device (EN 143). P1 (filters at least 80 % of airborne particles, colour code: White). 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.

1,6-Hexanediol $\geq 96\%$, for synthesis

article number: 1CP5

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	solid
Form	scales
Colour	colourless
Odour	odourless
Melting point/freezing point	39,5 – 42,1 °C (ECHA)
Boiling point or initial boiling point and boiling range	250 °C at 1.013 hPa (ECHA)
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	136 °C at 1.013 hPa (ECHA)
Auto-ignition temperature	320 °C at 1.013 hPa (ECHA) (relative self-ignition temperature for solids)
Decomposition temperature	not relevant
pH (value)	5 – 7 (in aqueous solution: 500 g/l, 20 °C)
Kinematic viscosity	not relevant
<u>Solubility(ies)</u>	
Water solubility	1.000 g/l (ECHA)
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	0 (25 °C) (ECHA)
Soil organic carbon/water (log KOC)	0 (ECHA)
Vapour pressure	0,001 hPa at 25 °C
<u>Density and/or relative density</u>	
Density	0,96 g/cm ³ at 20 °C (ECHA)
Relative vapour density	Information on this property is not available.
Bulk density	~530 kg/m ³
Particle characteristics	No data available.
<u>Other safety parameters</u>	
Oxidising properties	none

1,6-Hexanediol $\geq 96\%$, for synthesis

article number: 1CP5

9.2 Other information

Information with regard to physical hazard classes:

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

Other safety characteristics:

Temperature class (EU, acc. to ATEX)

T2
Maximum permissible surface temperature on the equipment: 300°C

SECTION 10: Stability and reactivity

10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

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

There are no specific conditions known which have to be avoided.

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	3.000 mg/kg	rat		ECHA
dermal	LD50	>2.500 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.

1,6-Hexanediol \geq 96 %, for synthesis

article number: **1CP5**

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.

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**

vomiting, nausea, gastrointestinal complaints

• **If in eyes**

causes slight to moderate irritation

• **If inhaled**

cough, headache

• **If on skin**

Frequently or prolonged contact with skin may cause dermal irritation

• **Other information**

none

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.

1,6-Hexanediol ≥96 %, for synthesis

article number: 1CP5

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	10.000 mg/l	fish	ECHA	96 h
EC50	>500 mg/l	aquatic invertebrates	ECHA	48 h
ErC50	5.940 mg/l	algae	ECHA	72 h

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
EC50	>10.000 mg/l	microorganisms	ECHA	17 h

12.2 Persistence and degradability

Theoretical Oxygen Demand: 2,302 mg/mg
Theoretical Carbon Dioxide: 2,234 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 (25 °C) (ECHA)
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12.4 Mobility in soil

Henry's law constant	0,041 Pa m ³ /mol at 25 °C (ECHA)
The Organic Carbon normalised adsorption coefficient	0 (ECHA)

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 ≥ 0,1%.

12.7 Other adverse effects

Data are not available.

1,6-Hexanediol ≥ 96 %, for synthesis

article number: 1CP5

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/packagings

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

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 <u>Information for each of the UN Model Regulations</u> | |
| 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. |

1,6-Hexanediol ≥ 96 %, for synthesis

article number: 1CP5

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		

Deco-Paint Directive

VOC content	100 %
VOC content	960 g/l

Industrial Emissions Directive (IED)

VOC content	0 %
VOC content	0 g/l

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

1,6-Hexanediol ≥96 %, for synthesis

article number: **1CP5**

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
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

Legend

AIIC	Australian Inventory of Industrial Chemicals
CICR	Chemical Inventory and Control Regulation
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

According to REACH, Article 14 (1) a chemical safety assessment has been carried out for this substance or components of this mixture when the substance has been registered in quantities of 10 tonnes or more per year per registrant.

1,6-Hexanediol ≥96 %, for synthesis

article number: **1CP5**

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 (ED) at a concentration of ≥ 0,1%.	yes
14.8	Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information: Not subject to ADR, RID and ADN.		yes
15.1	VOC content: 100 % 960 g/l	VOC content: 100 %	yes
15.1		VOC content: 960 g/l	yes
15.1		National inventories: change in the listing (table)	yes
15.2	Chemical Safety Assessment: No Chemical Safety Assessment has been carried out for this substance.	Chemical safety assessment: According to REACH, Article 14 (1) a chemical safety assessment has been carried out for this substance or components of this mixture when the substance has been registered in quantities of 10 tonnes or more per year per registrant.	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
ErC50	≡ EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association

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



1,6-Hexanediol ≥ 96 %, for synthesis

article number: 1CP5

Abbr.	Descriptions of used abbreviations
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
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
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). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). 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.