

#### 1,3-Butanediol ≥99 %, for synthesis

article number: **7473** Version: **2.0 en** Replaces version of: 2017-02-21 Version: (1) date of compilation: 2017-02-21 Revision: 2022-01-25

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

## 1.1 Product identifier

Identification of the substance	<b>1,3-Butanediol</b> ≥99 %, for synthesis
Article number	7473
Registration number (REACH)	01-2119455875-25-xxxx
EC number	203-529-7
CAS number	107-88-0
Alternative name(s)	1,3-Butylene glycol

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

Relevant identified uses:

Laboratory chemical Laboratory and analytical use

Uses advised against:

Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household).

## **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 :Department Health, Safety and Environment sheet:

e-mail (competent person):

# sicherheit@carlroth.de

#### 1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	



## 1,3-Butanediol ≥99 %, for synthesis

article number: 7473

# **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

#### **Results of PBT and vPvB assessment**

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

# **SECTION 3: Composition/information on ingredients**

#### 3.1 Substances

Name of substance	1,3-Butanediol
Molecular formula	$C_4H_{10}O_2$
Molar mass	90,12 <sup>g</sup> / <sub>mol</sub>
REACH Reg. No	01-2119455875-25-xxxx
CAS No	107-88-0
EC No	203-529-7

# **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.

#### 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.



article number: 7473

- **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

# **SECTION 5: Firefighting measures**

## 5.1 Extinguishing media



## Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO<sub>2</sub>)

## Unsuitable extinguishing media

water jet

### 5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and 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

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.

## 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.



## 1,3-Butanediol ≥99 %, for synthesis

article number: 7473

# **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. Store in a dry place. Hygroscopic.

# Incompatible substances or mixtures

Observe hints for combined storage.

Protect against external exposure, such as

humidity

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.

#### **Environmental values**

Relevan	t PNECs and ot	her threshold levels		
End- point	Threshold level	Organism	Environmental com- partment	Exposure time
PNEC	1.804 <sup>mg</sup> / <sub>l</sub>	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)

# 8.2 Exposure controls

# Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.



# 1,3-Butanediol ≥99 %, for synthesis

article number: 7473

**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  $^{\circ}$ 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
Colour	colourless
Odour	odourless
Melting point/freezing point	-57 °C (ECHA)
Boiling point or initial boiling point and boiling range	209 °C at 1.013 hPa (ECHA)
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	1,9 vol% (LEL) - 12,6 vol% (UEL)
Flash point	115 °C at 1.013 hPa (ECHA)
Auto-ignition temperature	410 °C at 1.019 hPa (ECHA)
Decomposition temperature	not relevant
pH (value)	6 – 7 (in aqueous solution: 1 <sup>g</sup> / <sub>l</sub> , 20 °C)



# 1,3-Butanediol ≥99 %, for synthesis

Kinematic viscosity	131,3 <sup>mm²</sup> / <sub>s</sub> at 20 °C
Solubility(ies)	
Water solubility	(soluble)
Partition coefficient	
Partition coefficient n-octanol/water (log value):	-0,9 (pH value: 7,5, 25 °C) (ECHA)
Vapour pressure	<1 hPa at 20 °C
Density and/or relative density	
Density	1,004 <sup>g</sup> / <sub>cm³</sub> at 20 °C (ECHA)
Relative vapour density	3,11 (air = 1)
Particle characteristics	not relevant (liquid)
Other safety parameters	
Oxidising properties	none
Other information	
Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
Other safety characteristics:	
Surface tension	72,6 <sup>mN</sup> / <sub>m</sub> (20 °C) (ECHA)
Refractive index	1,439 – 1,441
Temperature class (EU, acc. to ATEX)	T2 Maximum permissible surface temperature on the equipment: 300°C

# **SECTION 10: Stability and reactivity**

# 10.1 Reactivity

9.2

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, Acid halides

#### 10.4 Conditions to avoid



article number: 7473

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
dermal	LD50	>20.000 <sup>mg</sup> / <sub>kg</sub>	rabbit		TOXNET
oral	LD50	22.800 <sup>mg</sup> / <sub>kg</sub>	rat		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.

#### 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



article number: 7473

If swallowed

vomiting, nausea

## • If in eyes

slightly irritant but not relevant for classification

## • If inhaled

Data are not available.

## • If on skin

Frequently or prolonged contact with skin may cause dermal irritation

## Other information

none

- **11.2 Endocrine disrupting properties** Not listed.
- 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	>100 <sup>mg</sup> / <sub>l</sub>	fish	ECHA	96 h	
EC50	>1.000 <sup>mg</sup> / <sub>l</sub>	aquatic invertebrates	ECHA	48 h	
ErC50	>1.070 <sup>mg</sup> / <sub>l</sub>	algae	ECHA	72 h	

# Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
EC50	>85 <sup>mg</sup> /I	aquatic invertebrates	ECHA	21 d
LC50	>85 <sup>mg</sup> / <sub>l</sub>	aquatic invertebrates	ECHA	21 d

# Biodegradation

The substance is readily biodegradable.

#### 12.2 Process of degradability

Theoretical Oxygen Demand: 1,953 <sup>mg</sup>/<sub>mg</sub> Theoretical Carbon Dioxide: 1,953 <sup>mg</sup>/<sub>mg</sub>



article number: 7473

Process of degradability			
Process	Degradation rate	Time	
carbon dioxide generation	81 %	29 d	

#### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW) -0,9 (pH value: 7,5, 25 °C) (ECHA)	
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#### 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** Not listed.

#### 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.

#### 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. Waste catalogue ordinance (Germany).

#### 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 or ID number
- 14.2 UN proper shipping name
- 14.3 Transport hazard class(es)
- 14.4 Packing group
- 14.5 Environmental hazards

not subject to transport regulations

not assigned

none

not assigned

non-environmentally hazardous acc. to the dangerous goods regulations



article number: **7473** 

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
  - Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) Additional information

Not subject to ADR, RID and ADN.

**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 ap- plication of lower and upper-tier re- quirements	Notes
	not assigned		

#### **Deco-Paint Directive**

VOC content	100 % , 1.004 <sup>g</sup> / <sub>1</sub>

#### Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	1.004 <sup>g</sup> / <sub>l</sub>

# 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



article number: 7473

#### 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	AICS	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

Legend

AICS	Australian Inventory of Chemical Substances
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
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



# 1,3-Butanediol ≥99 %, for synthesis

article number: 7473

### 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)

Alignment to regulation: Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU

#### Restructuring: section 9, section 14

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
2.2	Signal word: not required		yes
2.3	Other hazards: There is no additional information.	Other hazards	yes
2.3		Results of PBT and vPvB assessment: According to the results of its assessment, this substance is not a PBT or a vPvB.	yes

#### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de naviga- tion intérieures (European Agreement concerning the International Carriage of Dangerous Goods by In- land Waterways)
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concern- ing 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)
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 identi- fier of substances commercially available within the EU (European Union)
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 Na- tions
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



#### article number: 7473

Abbr.	Descriptions of used abbreviations
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
LEL	Lower explosion limit (LEL)
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 (Regula- tions concerning the International carriage of Dangerous goods by Rail)
SVHC	Substance of Very High Concern
UEL	Upper explosion limit (UEL)
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.

Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN). 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.