according to Regulation (EC) No. 1907/2006 (REACH)

# ROTH

# 2,2-Dimethyl-1,3-propanediol ≥99 %, for synthesis

article number: **7349** date of compilation: 2021-02-03 Version: **1.0 en** 

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

# 1.1 Product identifier

Identification of the substance **2,2-Dimethyl-1,3-propanediol** ≥99 %, for syn-

thesis

Article number 7349

Registration number (REACH) 01-2119480396-30-xxxx

EC number 204-781-0 CAS number 126-30-7

# 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:

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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	

# **SECTION 2: Hazards identification**

# 2.1 Classification of the substance or mixture

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

Sect	ion	Hazard class	Cat- egory	Hazard class and category	Hazard statement
3.	3	Serious eye damage/eye irritation	1	Eye Dam. 1	H318

For full text of abbreviations: see SECTION 16

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### 2.2 Label elements

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

Signal word Danger

**Pictograms** 

GHS05



# **Hazard statements**

H318 Causes serious eye damage

# **Precautionary statements**

# **Precautionary statements - prevention**

P280 Wear protective clothing/eye protection

# **Precautionary statements - response**

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact

lenses, if present and easy to do. Continue rinsing

P310 Immediately call a doctor

# Labelling of packages where the contents do not exceed 125 ml

Signal word: Danger

Symbol(s)



H318 Causes serious eye damage.

P280 Wear protective clothing/eye protection.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to

do. Continue rinsing.

P310 Immediately call a doctor.

# 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 2,2-Dimethyl-1,3-propanediol

Molecular formula  $C_5H_{12}O_2$  Molar mass  $104,2\,^g/_{mol}$ 

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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. 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

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and 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

Risk of blindness, Risk of serious damage to eyes

# 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, 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**

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.

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# **SECTION 6: Accidental release measures**

# 6.1 Personal precautions, protective equipment and emergency procedures



# For non-emergency personnel

Avoid contact with skin, eyes and clothes. Do not breathe dust.

# 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. Take up mechanically.

# Advice on how to clean up a spill

Take up mechanically. Control of dust.

# 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

Provision of sufficient ventilation. Avoid dust formation.

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

Removal of dust deposits.

# Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

# 7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place. Keep container tightly closed. Hygroscopic solid.

### **Incompatible substances or mixtures**

Observe hints for combined storage.

# Consideration of other advice

# **Ventilation requirements**

Use local and general ventilation.

# Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C

# 7.3 Specific end use(s)

No information available.

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# SECTION 8: Exposure controls/personal protection

### **Control parameters** 8.1

# **National limit values**

# **Occupational exposure limit values (Workplace Exposure Limits)**

Coun	Name of agent	CAS No	Identifi- er	TWA [mg/ m³]	STEL [mg/ m³]	Ceil- ing-C [mg/ m³]	Nota- tion	Source
GB	dust		WEL	10			i	EH40/2005
GB	dust		WEL	4			r	EH40/2005

Notation

Ceiling value is a limit value above which exposure should not occur Inhalable fraction Ceiling-C

Respirable fraction

**STEL** 

Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)
Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 **TWA** 

hours time-weighted average (unless otherwise specified)

### **Human health values**

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

### **Environmental values**

# **Relevant PNECs and other threshold levels**

End- point	Threshold level	Organism	Environmental com- partment	Exposure time
PNEC	5 <sup>mg</sup> / <sub>l</sub>	aquatic organisms	freshwater	short-term (single instance)
PNEC	0,5 <sup>mg</sup> / <sub>l</sub>	aquatic organisms	marine water	short-term (single instance)
PNEC	20 <sup>mg</sup> / <sub>l</sub>	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	18,5 <sup>mg</sup> / <sub>kg</sub>	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	1,85 <sup>mg</sup> / <sub>kg</sub>	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0,77 <sup>mg</sup> / <sub>kg</sub>	terrestrial organisms	soil	short-term (single instance)

### 8.2 **Exposure controls**

Individual protection measures (personal protective equipment)

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# **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. 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. The times are approximate values from measurements at 22 °C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

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

# **Environmental exposure controls**

Keep away from drains, surface and ground water.

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# **SECTION 9: Physical and chemical properties**

# 9.1 Information on basic physical and chemical properties

Physical state solid

Form powder, crystalline

Colour white

Odour mild sweet

Melting point/freezing point 127 – 130 °C

Boiling point or initial boiling point and boiling 209 °C at 1.013 hPa

range

Flammability this material is combustible, but will not ignite

readily

Lower and upper explosion limit 1,4 vol% - 18,8 vol%

Flash point 103 °C (c.c.)
Auto-ignition temperature not determined
Decomposition temperature not relevant
pH (value) not applicable
Kinematic viscosity not relevant

Solubility(ies)

Water solubility 830 <sup>g</sup>/<sub>l</sub> at 20 °C

Partition coefficient

Partition coefficient n-octanol/water (log value): -0,16 (25 °C) (exp. TOXNET)

Vapour pressure <1 hPa at 20 °C

Density  $1,07 \, {}^{9}/_{cm^3}$  at 20  ${}^{\circ}$ C

Particle characteristics no data available

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard hazard classes acc. to GHS

classes: (physical hazards): not relevant

Other safety characteristics:

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

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

Moisture-sensitive. Hygroscopic solid.

# 10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser

### 10.4 Conditions to avoid

Humidity.

# 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)

# **Acute toxicity**

Shall not be classified as acutely toxic.

_			•	• .
Αcι	140	+~	~1~	
MLL	,,,		X II	.II.V

Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	>6.400 <sup>mg</sup> / <sub>kg</sub>	rat		ECHA
dermal	LD50	>4.000 <sup>mg</sup> / <sub>kg</sub>	guinea pig		ECHA

### Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

# Serious eye damage/eye irritation

Causes serious eye damage.

# 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).

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# 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

Causes serious eye damage, risk of blindness

### If inhaled

Data are not available.

### • If on skin

Frequently or prolonged contact with skin may cause dermal irritation

### Other information

none

# **SECTION 12: Ecological information**

# 12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

# Endpoint Value Species Exposure time LC50 >10.000 mg/<sub>I</sub> fish 48 h EC50 >500 mg/<sub>I</sub> aquatic invertebrates 48 h

# **Biodegradation**

The substance is readily biodegradable. The relevant substances of the mixture are readily biodegradable.

# 12.2 Process of degradability

Theoretical Oxygen Demand with nitrification: 2,151 <sup>mg</sup>/<sub>mg</sub> Theoretical Oxygen Demand without nitrification: 2,151 <sup>mg</sup>/<sub>mg</sub>

Theoretical Carbon Dioxide: 2,113 mg/mg

# **Process of degradability**

Process	Degradation rate	Time
biotic/abiotic	<5 %	35 d
carbon dioxide generation	>80 - <90 %	28 d

# 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

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n-octanol/water (log KOW)	-0,16 (25 °C) (Exp. TOXNET)
BCF	<9 (ECHA)

# 12.4 Mobility in soil

Henry's law constant	0 <sup>Pa m³</sup> / <sub>mol</sub> (ECHA)

### 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



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.

### 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 n	umber or ID number	not subject to transport regulations
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**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 dan-

gerous 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.

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# Information for each of the UN Model Regulations

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

not assigned

**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/	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 (2004/42/EC)**

VOC content	100 % 1.070 <sup>g</sup> / <sub>I</sub>

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

VOC content	100 %
VOC content	1.070 <sup>g</sup> / <sub>l</sub>

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

**Water Framework Directive (WFD)** 

not listed

Regulation 98/2013/EU on the marketing and use of explosives precursors

not listed

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Regulation 111/2005/EC laying down rules for the monitoring of trade between the Community and third countries in drug precursors

not listed

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

not listed

Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)

not listed

### **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

Australian Inventory of Chemical Substances Chemical Inventory and Control Regulation List of Existing and New Chemical Substances (CSCL-ENCS) AICS CICR

CSCL-ENCS

CSCL-ENCS

List of Existing and New Chemical Substances (CSCL-ENCS)

Domestic Substances List (DSL)

ECSI EC Substance Inventory (EINECS, ELINCS, NLP)

IECSC Inventory of Existing Chemical Substances Produced or Imported in China 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 Substances Inventory

TCSI TSCA Taiwan Chemical Substance Inventory **Toxic Substance Control Act** 

# 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 naviga- tion intérieures (European Agreement concerning the International Carriage of Dangerous Goods by In- land Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	Ceiling value
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)
EH40/2005	EH40/2005 Workplace exposure limits (http://www.nationalarchives.gov.uk/doc/open-government-licence/)
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
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
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
STEL	Short-term exposure limit
SVHC	Substance of Very High Concern
TWA	Time-weighted average

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Abbr.	Descriptions of used abbreviations
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative
WEL	Workplace exposure limit

# 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).

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

Code	Text
H318	Causes serious eye damage.

# **Disclaimer**

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

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