

Safety data sheet

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



1-Heptanol ≥99 %, for synthesis

article number: **3827**

Version: **3.0 en**

Replaces version of: 2021-10-22

Version: (2)

date of compilation: 2015-08-25

Revision: 2024-03-02

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

1.1 Product identifier

Identification of the substance	1-Heptanol ≥99 %, for synthesis
Article number	3827
EC number	203-897-9
CAS number	111-70-6

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 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 Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.3	Serious eye damage/eye irritation	2	Eye Irrit. 2	H319

For full text of abbreviations: see SECTION 16

2.2 Label elements

Safety data sheet

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



1-Heptanol $\geq 99\%$, for synthesis

article number: **3827**

Labelling

Signal word

Warning

Pictograms

GHS07



Hazard statements

H319 Causes serious eye irritation

Precautionary statements

Precautionary statements - prevention

P264 Wash thoroughly after handling
P280 Wear protective gloves/protective clothing/eye protection/face 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
P337+P313 If eye irritation persists: Get medical advice/attention

2.3 Other hazards

This material is combustible, but will not ignite readily.

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-Heptanol
Molecular formula	$C_7H_{16}O$
Molar mass	$116,2 \text{ g/mol}$
CAS No	111-70-6
EC No	203-897-9

Safety data sheet

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



1-Heptanol $\geq 99\%$, for synthesis

article number: 3827

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air.

Following skin contact

Rinse skin with water/shower.

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

Following ingestion

Let water be drunk in little sips (dilution effect). Call a doctor.

4.2 Most important symptoms and effects, both acute and delayed

Irritation

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, 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. 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 (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.

Safety data sheet

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



1-Heptanol ≥99 %, for synthesis

article number: **3827**

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 vapour/spray.

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.

Advice on how to clean up a spill

Absorb with liquid-binding material (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

Provision of sufficient ventilation.

Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

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

Keep container tightly closed.

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.

Safety data sheet

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



1-Heptanol ≥99 %, for synthesis

article number: 3827

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	35,26 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	0,027 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0,003 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	10 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,22 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,022 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0,028 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



Safety data sheet

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



1-Heptanol $\geq 99\%$, for synthesis

article number: 3827

• 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

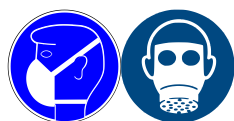
• breakthrough times of the glove material

>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: 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
Colour	colourless
Odour	characteristic
Melting point/freezing point	-34,6 °C
Boiling point or initial boiling point and boiling range	179,4 °C at 1.013 hPa (ECHA)
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	0,9 vol% (LEL)
Flash point	76 °C at 1.013 hPa
Auto-ignition temperature	292 °C at 992 hPa (ECHA)
Decomposition temperature	not relevant
pH (value)	not determined

Safety data sheet

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



1-Heptanol ≥99 %, for synthesis

article number: **3827**

Kinematic viscosity	8,902 mm ² /s at 20 °C
Dynamic viscosity	7,3 mPa s at 20 °C
<u>Solubility(ies)</u>	
Water solubility	1,63 g/l at 20 °C (ECHA)
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	2,2 (20 °C) (ECHA)
Soil organic carbon/water (log KOC)	1,66 (ECHA)
Vapour pressure	0,7 hPa at 20 °C
<u>Density and/or relative density</u>	
Density	0,82 g/cm ³ at 20 °C
Relative vapour density	4,01 (air = 1)
Particle characteristics	not relevant (liquid)
<u>Other safety parameters</u>	
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:	
Surface tension	41 mN/m (19,3 °C) (ECHA)

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

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

Safety data sheet

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



1-Heptanol ≥99 %, for synthesis

article number: 3827

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 toxicological effects

Classification acc. to GHS

Acute toxicity

Shall not be classified as acutely toxic.

GHS of the United Nations, annex 4. May be harmful in contact with skin.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	6.200 mg/kg	rat		ECHA
dermal	LD50	>2.000 mg/kg	rabbit		ECHA

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Causes serious eye irritation.

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

Data are not available.

• If in eyes

Causes serious eye irritation

Safety data sheet

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



1-Heptanol ≥99 %, for synthesis

article number: 3827

• If inhaled

Data are not available.

• If on skin

Data are not available.

• 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.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	17,6 mg/l	fish	ECHA	96 h
EC50	94 mg/l	aquatic invertebrates	ECHA	24 h
ErC50	32,7 mg/l	algae	ECHA	72 h

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
EC50	>100 mg/l	microorganisms	ECHA	3 h

12.2 Persistence and degradability

Theoretical Oxygen Demand: 2,891 mg/mg
Theoretical Carbon Dioxide: 2,651 mg/mg

Biodegradation

The substance is readily biodegradable.

Process of degradability		
Process	Degradation rate	Time
oxygen depletion	84 %	28 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

Safety data sheet

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



1-Heptanol $\geq 99\%$, for synthesis

article number: **3827**

n-octanol/water (log KOW)	2,2 (20 °C) (ECHA)
BOD5/COD	56,3 (HSDB)

12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	1,66 (ECHA)
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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



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

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.

Properties of waste which render it hazardous

HP 4 irritant - skin irritation and eye damage

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

Safety data sheet

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



1-Heptanol ≥99 %, for synthesis

article number: 3827

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)

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	820 g/l

Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	820 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

Safety data sheet

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



1-Heptanol ≥99 %, for synthesis

article number: 3827

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

National regulations(GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

Restrictions according to GB REACH, Annex 17

Dangerous substances with restrictions (GB REACH, Annex 17)			
Name of substance	Name acc. to inventory	CAS No	No
1-Heptanol	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		3

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

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

Safety data sheet

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



1-Heptanol ≥99 %, for synthesis

article number: 3827

Legend

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
2.2	Labelling of packages where the contents do not exceed 125 ml: Signal word: Warning		yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
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	Restrictions according to REACH, Annex XVII		yes
15.1		Dangerous substances with restrictions (REACH, Annex XVII): change in the listing (table)	yes
15.1	List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list: Not listed.		yes
15.1	VOC content: 100 % , 820 g/l	VOC content: 100 %	yes
15.1		VOC content: 820 g/l	yes
15.1		National regulations(GB)	yes
15.1		List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list: not listed	yes
15.1		Restrictions according to GB REACH, Annex 17	yes
15.1		Dangerous substances with restrictions (GB REACH, Annex 17): change in the listing (table)	yes
15.1		National inventories: change in the listing (table)	yes

Safety data sheet

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



1-Heptanol ≥99 %, for synthesis

article number: 3827

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)
BOD	Biochemical Oxygen Demand
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
COD	Chemical oxygen demand
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
GB REACH	The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended)
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
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 (Regulations concerning the International carriage of Dangerous goods by Rail)
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Safety data sheet

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



1-Heptanol ≥99 %, for synthesis

article number: **3827**

Key literature references and sources for data

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).

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

Code	Text
H319	Causes serious eye irritation.

Disclaimer

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