

# Safety data sheet

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



**Heptane (isomers) >=98,5 %, for synthesis ≥98,5 %, for synthesis**

article number: **7725**

Version: **2.0 en**

Replaces version of: 2021-05-18

Version: (1)

date of compilation: 2021-05-17

Revision: 2024-03-04

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

### 1.1 Product identifier

Identification of the substance	<b>Heptane (isomers) &gt;=98,5 %, for synthesis ≥98,5 %, for synthesis</b>
Article number	7725
Index No (GB CLP)	649-328-00-1
EC number	927-510-4
CAS number	64742-49-0
Alternative name(s)	Hydrocarbons, C <sub>7</sub> , n-alkanes, isoalkanes, cyclics

### 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 products which come into contact with foodstuffs. Do not use for private purposes (household). Food, drink and animal feeding-stuffs.

### 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](mailto:sicherheit@carlroth.de)

**Website:** [www.carlroth.de](http://www.carlroth.de)

Competent person responsible for the safety data sheet: Department Health, Safety and Environment

**e-mail (competent person):** [sicherheit@carlroth.de](mailto: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	

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## 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
2.6	Flammable liquid	2	Flam. Liq. 2	H225
3.2	Skin corrosion/irritation	2	Skin Irrit. 2	H315
3.8D	Specific target organ toxicity - single exposure (narcotic effects, drowsiness)	3	STOT SE 3	H336
3.10	Aspiration hazard	1	Asp. Tox. 1	H304
4.1C	Hazardous to the aquatic environment - chronic hazard	2	Aquatic Chronic 2	H411

The classification as a carcinogen or mutagen is not required. The substance contains less than 0,1 % w/w benzene (EINECS No 200-753-7). For full text of abbreviations: see SECTION 16

### The most important adverse physicochemical, human health and environmental effects

The product is combustible and can be ignited by potential ignition sources. Spillage and fire water can cause pollution of watercourses.

### 2.2 Label elements

#### Labelling

#### Signal word

**Danger**

#### Pictograms

GHS02, GHS07,  
GHS08, GHS09



#### Hazard statements

H225 Highly flammable liquid and vapour  
H304 May be fatal if swallowed and enters airways  
H315 Causes skin irritation  
H336 May cause drowsiness or dizziness  
H411 Toxic to aquatic life with long lasting effects

#### Precautionary statements

##### Precautionary statements - prevention

P210 Keep away from heat, sparks, open flames, hot surfaces. No smoking  
P273 Avoid release to the environment

##### Precautionary statements - response

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P331 Do NOT induce vomiting

##### Precautionary statements - storage

P403+P235 Store in a well-ventilated place. Keep cool

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## 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

"UVCB substance" (substance of unknown or variable composition).

Name of substance	Hydrocarbons, C <sub>7</sub> , n-alkanes, isoalkanes, cyclics
CAS No	64742-49-0
EC No	927-510-4
Index No (GB CLP)	649-328-00-1

#### Impurities/additives/constituents:

Name of substance	Identifier	Wt%
n-Heptane	CAS No 142-82-5  EC No 205-563-8  Index No 601-008-00-2	30 - 40

#### Remarks

For full text of abbreviations: see SECTION 16

## 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 case of skin irritation, consult a physician.

#### Following eye contact

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

#### Following ingestion

Call a physician immediately. Observe aspiration hazard if vomiting occurs.

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## 4.2 Most important symptoms and effects, both acute and delayed

Aspiration hazard, Irritation, Dizziness, Drowsiness, Narcosis

## 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. In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours may form explosive mixtures with air.

#### Hazardous combustion products

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), May produce toxic fumes of carbon monoxide if burning.

### 5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Do not allow firefighting water to enter drains or water courses. 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

Use personal protective equipment as required. Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

### 6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it. If substance has entered a water course or sewer, inform the responsible authority.

### 6.3 Methods and material for containment and cleaning up

#### Advice on how to contain a spill

Covering of drains.

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## **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.

Take precautionary measures against static discharge. Due to danger of explosion, prevent leakage

of vapours into cellars, flues and ditches.

### **Measures to protect the environment**

Avoid release to the environment.

### **Advice on general occupational hygiene**

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs. When using do not smoke.

### **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:**

Ground/bond container and receiving equipment.

### **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

### 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	2.085 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	300 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

Relevant DNELs of components						
Name of substance	CAS No	End-point	Threshold level	Protection goal, route of exposure	Used in	Exposure time
n-Heptane	142-82-5	DNEL	2.085 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - systemic effects
n-Heptane	142-82-5	DNEL	300 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

### 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. 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.

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- **type of material**

NBR: acrylonitrile-butadiene rubber

- **material thickness**

0,4 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.

Flame-retardant protective clothing.

### Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of  $> 65\text{ °C}$ , 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	clear - colourless
Odour	characteristic
Melting point/freezing point	$< -90\text{ °C}$
Boiling point or initial boiling point and boiling range	$89 - 97\text{ °C}$ at 100 kPa (ECHA)
Flammability	flammable liquid in accordance with GHS criteria
Lower and upper explosion limit	0,6 vol% (LEL) - 7 vol% (UEL)
Flash point	$< 0\text{ °C}$ at 1 atm (ECHA)
Auto-ignition temperature	$> 200\text{ °C}$ at 1 atm (ECHA) (auto-ignition temperature (liquids and gases))
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	$0,67\text{ mm}^2/\text{s}$ at $20\text{ °C}$
<u>Solubility(ies)</u>	
Water solubility	$0,014\text{ g/l}$ at $25\text{ °C}$ (ECHA)
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	3,6 (pH value: 7, $20\text{ °C}$ ) (ECHA)

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Vapour pressure	6 kPa at 20 °C
<u>Density and/or relative density</u>	
Density	0,7 – 0,73 g/cm <sup>3</sup> at 15 °C (ECHA)
Relative vapour density	Information on this property is not available.
Particle characteristics	not relevant (liquid)
<u>Other safety parameters</u>	
Oxidising properties	none
<b>9.2 Other information</b>	
Information with regard to physical hazard classes:	There is no additional information.
Other safety characteristics:	
Surface tension	20,7 mN/m (25 °C) (ECHA)

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

It's a reactive substance. Risk of ignition. Vapours may form explosive mixtures with air.

#### If heated

Risk of ignition.

### 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, Chlorine, Phosphorus

### 10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

### 10.5 Incompatible materials

Rubber articles, different plastics

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.



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## 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 or if inhaled.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
inhalation: vapour	LC50	$>23,3 \text{ mg/l/4h}$	rat		ECHA
dermal	LD50	$>2.800 - 3.100 \text{ mg/kg}$	rat		ECHA

#### Acute toxicity of components

Name of substance	CAS No	Exposure route	Endpoint	Value	Species
n-Heptane	142-82-5	oral	LD50	$>5.000 \text{ mg/kg}$	rat
n-Heptane	142-82-5	inhalation: vapour	LC50	$>29,29 \text{ mg/l/4h}$	rat
n-Heptane	142-82-5	dermal	LD50	$>2.000 \text{ mg/kg}$	rabbit

#### Skin corrosion/irritation

Causes skin irritation.

#### 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

May cause drowsiness or dizziness.

#### Specific target organ toxicity - repeated exposure

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

#### Aspiration hazard

May be fatal if swallowed and enters airways.

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## Symptoms related to the physical, chemical and toxicological characteristics

### • If swallowed

gastrointestinal complaints, nausea, vomiting, aspiration hazard, varying degrees of pulmonary injury

### • If in eyes

slightly irritant but not relevant for classification

### • If inhaled

vertigo, Dyspnoea, fatigue, narcosis

### • If on skin

causes skin irritation

### • Other information

none

## 11.2 Endocrine disrupting properties

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

## 11.3 Information on other hazards

There is no additional information.

## SECTION 12: Ecological information

### 12.1 Toxicity

Toxic to aquatic life with long lasting effects.

Aquatic toxicity (acute) of components					
Name of substance	CAS No	Endpoint	Value	Species	Exposure time
n-Heptane	142-82-5	EC50	0,64 mg/l	aquatic invertebrates	48 h

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
EC50	0,23 mg/l	aquatic invertebrates	ECHA	21 d

Aquatic toxicity (chronic) of components					
Name of substance	CAS No	Endpoint	Value	Species	Exposure time
n-Heptane	142-82-5	EC50	0,23 mg/l	aquatic invertebrates	21 d

### 12.2 Persistence and degradability

#### Biodegradation

The substance is readily biodegradable.

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Process of degradability		
Process	Degradation rate	Time
oxygen depletion	83 %	16 d

Degradability of components						
Name of substance	CAS No	Process	Degradation rate	Time	Method	Source
n-Heptane	142-82-5	oxygen depletion	28,2 %	2 d		ECHA

## 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	3,6 (pH value: 7, 20 °C) (ECHA)
---------------------------	---------------------------------

Bioaccumulative potential of components				
Name of substance	CAS No	BCF	Log KOW	BOD5/COD
n-Heptane	142-82-5	552	4,5	

## 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



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. Avoid release to the environment. Refer to special instructions/safety data sheets.

#### Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used. 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.

### Properties of waste which render it hazardous

**HP 3** flammable

**HP 4** irritant - skin irritation and eye damage

**HP 5** specific target organ toxicity (STOT)/aspiration toxicity

**HP 14** ecotoxic

## 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

ADRRID	UN 1206
IMDG-Code	UN 1206
ICAO-TI	UN 1206

### 14.2 UN proper shipping name

ADRRID	HEPTANES
IMDG-Code	HEPTANES
ICAO-TI	Heptanes

### 14.3 Transport hazard class(es)

ADRRID	3
IMDG-Code	3
ICAO-TI	3

### 14.4 Packing group

ADRRID	II
IMDG-Code	II
ICAO-TI	II

### 14.5 Environmental hazards

hazardous to the aquatic environment

### 14.6 Special precautions for user

Provisions for dangerous goods (ADR) should be complied within the premises.

### 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

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## Agreement concerning the International Carriage of Dangerous Goods by Road (ADR) Additional information

Proper shipping name	HEPTANES
Particulars in the transport document	UN1206, HEPTANES, 3, II, (D/E), environmentally hazardous
Classification code	F1
Danger label(s)	3, "Fish and tree"
 	
Environmental hazards	yes (hazardous to the aquatic environment)
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
Transport category (TC)	2
Tunnel restriction code (TRC)	D/E
Hazard identification No	33
<b>Emergency Action Code</b>	3YE

## Regulations concerning the International Carriage of Dangerous Goods by Rail (RID) Additional information

Classification code	F1
Danger label(s)	3, "Fish and tree"
 	
Environmental hazards	Yes Hazardous to water
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
Transport category (TC)	2
Hazard identification No	33

## International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name	HEPTANES
Particulars in the shipper's declaration	UN1206, HEPTANES, 3, II, $<0^{\circ}\text{C}$ c.c., MARINE POLLUTANT
Marine pollutant	yes (P) (hazardous to the aquatic environment)
Danger label(s)	3, "Fish and tree"
 	
Special provisions (SP)	-
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L


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EmS	F-E, S-D
Stowage category	B
<b>International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information</b>	
Proper shipping name	Heptanes
Particulars in the shipper's declaration	UN1206, Heptanes, 3, II
Environmental hazards	yes (hazardous to the aquatic environment)
Danger label(s)	3
	
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L

## 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
E2	environmental hazards (hazardous to the aquatic environment, cat. 2)	200                      500	57)

##### Notation

57) Hazardous to the Aquatic Environment in category Chronic 2

##### Deco-Paint Directive

VOC content	100 %
VOC content	730 g/l

##### Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	730 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

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## Water Framework Directive (WFD)

List of pollutants (WFD)				
Name of substance	Name acc. to inventory	CAS No	Listed in	Remarks
Hydrocarbons, C <sub>7</sub> , n-alkanes, isoalkanes, cyclics	Substances and preparations, or the breakdown products of such, which have been proved to possess carcinogenic or mutagenic properties or properties which may affect steroidogenic, thyroid, reproduction or other endocrine-related functions in or via the aquatic environment		a)	

### Legend

a) Indicative list of the main pollutants

### 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

### 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
Hydrocarbons, C <sub>7</sub> , n-alkanes, isoalkanes, cyclics	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		3
Hydrocarbons, C <sub>7</sub> , n-alkanes, isoalkanes, cyclics	carcinogenic		28
Hydrocarbons, C <sub>7</sub> , n-alkanes, isoalkanes, cyclics	germ cell mutagenic (mutagenic)		29
Hydrocarbons, C <sub>7</sub> , n-alkanes, isoalkanes, cyclics	flammable / pyrophoric		40

### 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.

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## 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
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
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
2.2	Labelling of packages where the contents do not exceed 125 ml: Signal word: Danger		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
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes



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**Heptane (isomers) >=98,5 %, for synthesis ≥98,5 %, for synthesis**

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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
14.1	ADR/RID/ADN: UN 3295	ADRRID: UN 1206	yes
14.1	IMDG-Code: UN 3295	IMDG-Code: UN 1206	yes
14.1	ICAO-TI: UN 3295	ICAO-TI: UN 1206	yes
14.2	ADR/RID/ADN: HYDROCARBONS, LIQUID, N.O.S.	ADRRID: HEPTANES	yes
14.2	IMDG-Code: HYDROCARBONS, LIQUID, N.O.S.	IMDG-Code: HEPTANES	yes
14.2	ICAO-TI: Hydrocarbons, liquid, n.o.s.	ICAO-TI: Heptanes	yes
14.8	Proper shipping name: HYDROCARBONS, LIQUID, N.O.S.	Proper shipping name: HEPTANES	yes
14.8	Particulars in the transport document: UN3295, HYDROCARBONS, LIQUID, N.O.S., 3, II, (D/E), environmentally hazardous, special provision 640D	Particulars in the transport document: UN1206, HEPTANES, 3, II, (D/E), environmentally hazardous	yes
14.8	Special provisions (SP): 640D		yes
14.8		Regulations concerning the International Carriage of Dangerous Goods by Rail (RID)Additional information	yes
14.8		Classification code: F1	yes
14.8		Danger label(s): 3, "Fish and tree"	yes
14.8		Danger label(s): change in the listing (table)	yes
14.8		Environmental hazards: Yes Hazardous to water	yes
14.8		Excepted quantities (EQ): E2	yes
14.8		Limited quantities (LQ): 1 L	yes
14.8		Transport category (TC): 2	yes
14.8		Hazard identification No: 33	yes
14.8	Proper shipping name: HYDROCARBONS, LIQUID, N.O.S.	Proper shipping name: HEPTANES	yes
14.8	Particulars in the shipper's declaration: UN3295, HYDROCARBONS, LIQUID, N.O.S., 3, II, <0°C c.c., MARINE POLLUTANT	Particulars in the shipper's declaration: UN1206, HEPTANES, 3, II, <0°C c.c., MARINE POLLUTANT	yes

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Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
14.8	Marine pollutant: yes (hazardous to the aquatic environment)	Marine pollutant: yes (P) (hazardous to the aquatic environment)	yes
14.8	Proper shipping name: Hydrocarbons, liquid, n.o.s.	Proper shipping name: Heptanes	yes
14.8	Particulars in the shipper's declaration: UN3295, Hydrocarbons, liquid, n.o.s., 3, II	Particulars in the shipper's declaration: UN1206, Heptanes, 3, II	yes
14.8	Special provisions (SP): A3		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 % 730 g/l	VOC content: 100 %	yes
15.1		VOC content: 730 g/l	yes
15.1	Water Framework Directive (WFD): not listed	Water Framework Directive (WFD)	yes
15.1		List of pollutants (WFD): change in the listing (table)	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		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.	yes
15.1		National inventories: change in the listing (table)	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)
BCF	Bioconcentration factor
BOD	Biochemical Oxygen Demand

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Abbr.	Descriptions of used abbreviations
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
EmS	Emergency Schedule
GB CLP	The Chemicals (Health and Safety) and Genetically Modified Organisms (Contained Use) (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/720 (as amended)
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
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
index No	The Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
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)
log KOW	n-Octanol/water
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
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)
UEL	Upper explosion limit (UEL)
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

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**Heptane (isomers)  $\geq 98,5$  %, for synthesis  $\geq 98,5$  %, for synthesis**

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## 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
H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
H411	Toxic to aquatic life with long lasting effects.

## Disclaimer

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