

Safety data sheet

Safe Work Australia - Code of Practice



n-Heptane ≥99 %, for synthesis

article number: **8654**
Version: **GHS 2.0 en**
Replaces version of: 2016-02-22
Version: (GHS 1)

date of compilation: 2016-02-22
Revision: 2019-09-25

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

1.1 Product identifier

Identification of the substance	n-Heptane
Article number	8654
Registration number (REACH)	01-2119457603-38-xxxx
Index No	601-008-00-2
EC number	205-563-8
CAS number	142-82-5

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

Identified uses: laboratory chemical
laboratory and analytical use

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
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 Westmead, NSW	131126	

Emergency information service

Poison Centre Munich: +49/(0)89 19240

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Safety data sheet

Safe Work Australia - Code of Practice



n-Heptane ≥99 %, for synthesis

article number: 8654

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
2.6	flammable liquid	(Flam. Liq. 2)	H225
3.2	skin corrosion/irritation	(Skin Irrit. 2)	H315
3.8D	specific target organ toxicity - single exposure (narcotic effects, drowsiness)	(STOT SE 3)	H336
3.10	aspiration hazard	(Asp. Tox. 1)	H304

The most important adverse physicochemical, human health and environmental effects

Narcotic effects.

2.2 Label elements

Labelling GHS

Signal word

Danger

Pictograms

GHS02, GHS07,
GHS08



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

Precautionary statements

Precautionary statements - prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

Precautionary statements - response

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P302+P352 IF ON SKIN: Wash with plenty of soap and water.
P331 Do NOT induce vomiting.
P370+P378 In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction.

Precautionary statements - storage

P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P403+P235 Store in a well-ventilated place. Keep cool.

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



Safety data sheet

Safe Work Australia - Code of Practice



n-Heptane $\geq 99\%$, for synthesis

article number: **8654**

H304	May be fatal if swallowed and enters airways.
P301+P310 P331	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. Do NOT induce vomiting.

2.3 Other hazards

There is no additional information.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	n-Heptane
Index No	601-008-00-2
Registration number (REACH)	01-2119457603-38-xxxx
EC number	205-563-8
CAS number	142-82-5
Molecular formula	C_7H_{16}
Molar mass	100.2 g/mol

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

Do NOT induce vomiting. Call a physician immediately. Observe aspiration hazard if vomiting occurs.

4.2 Most important symptoms and effects, both acute and delayed

Aspiration hazard, Irritation, Headache, Vertigo, Dizziness, Drowsiness, Narcosis

4.3 Indication of any immediate medical attention and special treatment needed

none

n-Heptane $\geq 99\%$, for synthesis

article number: 8654

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings
water spray, foam, dry extinguishing 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

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. Explosive properties.

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 (e.g. 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.

n-Heptane ≥99 %, for synthesis

article number: 8654

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation. Use extractor hood (laboratory).

- **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

Store in a well-ventilated place. 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.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Country	Name of agent	CAS No	Notation	Identifier	TWA [ppm]	TWA [mg/m ³]	STEL [ppm]	STEL [mg/m ³]	Source
AU	n-heptane	142-82-5		WES	400	1,640	500	2,050	WES

Notation

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)

TWA Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified)

n-Heptane ≥99 %, for synthesis

article number: 8654

Relevant DNELs/DMELs/PNECs and other threshold levels

• human health values

Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	2,085 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
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.

• type of material

NBR (Nitrile 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 °C, colour code: Brown).

n-Heptane ≥99 %, for synthesis

article number: **8654**

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

Appearance

Physical state	liquid (fluid)
Colour	colourless
Odour	like: Gasoline
Odour threshold	No data available

Other physical and chemical parameters

pH (value)	This information is not available.
Melting point/freezing point	-90.5 °C
Initial boiling point and boiling range	98.2 – 98.4 °C at 100 kPa
Flash point	-4 °C
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)
<u>Explosive limits</u>	
• lower explosion limit (LEL)	0.84 vol%
• upper explosion limit (UEL)	6.7 vol%
Explosion limits of dust clouds	not relevant
Vapour pressure	6.09 kPa at 25 °C
Density	0.69 g/cm ³ at 15 °C
Vapour density	3.46 (air = 1)
Bulk density	Not applicable
Relative density	Information on this property is not available.
<u>Solubility(ies)</u>	
Water solubility	2.4 mg/l at 25 °C
<u>Partition coefficient</u>	
n-octanol/water (log KOW)	4.5 (ECHA)
Soil organic carbon/water (log KOC)	2.38 (ECHA)
Auto-ignition temperature	204 °C - ECHA
Decomposition temperature	no data available
Viscosity	
• kinematic viscosity	0.641 mm ² /s at 20 °C
• dynamic viscosity	0.4423 cP

n-Heptane ≥99 %, for synthesis

article number: **8654**

Explosive properties	Shall not be classified as explosive
Oxidising properties	none

9.2 Other information

Surface tension	19.66 mN/m (25 °C)
-----------------	--------------------

SECTION 10: Stability and reactivity

10.1 Reactivity

Risk of ignition. Vapours can 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, Phosphorus, Chlorine

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.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Shall not be classified as acutely toxic.

Exposure route	Endpoint	Value	Species	Source
oral	LD50	>5,000 mg/kg	rat	ECHA
inhalation: vapour	LC50	>29.29 mg/l/4h	rat	ECHA
dermal	LD50	>2,000 mg/kg	rabbit	ECHA

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.

Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor as a reproductive toxicant

• Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Safety data sheet

Safe Work Australia - Code of Practice



n-Heptane ≥99 %, for synthesis

article number: 8654

• 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.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

aspiration hazard

• If in eyes

causes slight to moderate irritation

• If inhaled

headache, vertigo, dizziness, drowsiness, narcosis

• If on skin

Prolonged or repeated skin contact may cause removal of natural fat from the skin resulting in dermatitis (skin inflammation)

Other information

None

SECTION 12: Ecological information

12.1 Toxicity

acc. to 1272/2008/EC: Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
EC50	0.64 mg/l	aquatic invertebrates	ECHA	48 h

Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
EC50	0.23 mg/l	aquatic invertebrates	ECHA	21 d
NOEC	0.17 mg/l	aquatic invertebrates	ECHA	21 d

12.2 Process of degradability

Theoretical Oxygen Demand: 3.513 mg/mg
Theoretical Carbon Dioxide: 3.074 mg/mg

Process	Degradation rate	Time
oxygen depletion	28.2 %	2 d

12.3 Bioaccumulative potential

The substance fulfils the very bioaccumulative criterion.

n-octanol/water (log KOW)	4.5
BCF	552 (ECHA)

Safety data sheet

Safe Work Australia - Code of Practice



n-Heptane $\geq 99\%$, for synthesis

article number: 8654

12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient 2.38

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 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

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

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

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


13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions.

SECTION 14: Transport information

14.1	UN number	1206
14.2	UN proper shipping name	HEPTANES
	Hazardous ingredients	n-Heptane
14.3	Transport hazard class(es)	
	Class	3 (flammable liquids)
14.4	Packing group	II (substance presenting medium danger)
14.5	Environmental hazards	hazardous to the aquatic environment

n-Heptane ≥99 %, for synthesis

article number: **8654**

14.6 Special precautions for user

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

14.7 Transport in bulk according to Annex II of MARPOL and the IBC Code

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)

UN number	1206
Proper shipping name	HEPTANES
Particulars in the transport document	UN1206, HEPTANES, 3, II, (D/E), environmentally hazardous
Class	3
Classification code	F1
Packing group	II
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
Emergency Action Code	3YE

• International Maritime Dangerous Goods Code (IMDG)

UN number	1206
Proper shipping name	HEPTANES
Particulars in the shipper's declaration	UN1206, HEPTANES, 3, II, -4°C c.c., MARINE POLLUTANT
Class	3
Marine pollutant	yes (P) (hazardous to the aquatic environment)
Packing group	II
Danger label(s)	3 + "fish and tree"



Special provisions (SP)	-
Excepted quantities (EQ)	E2


Safety data sheet

Safe Work Australia - Code of Practice



n-Heptane ≥99 %, for synthesis

article number: 8654

Limited quantities (LQ)	1 L
EmS	F-E, S-D
Stowage category	B
• International Civil Aviation Organization (ICAO-IATA/DGR)	
UN number	1206
Proper shipping name	Heptanes
Particulars in the shipper's declaration	UN1206, Heptanes, 3, II
Class	3
Environmental hazards	yes (hazardous to the aquatic environment)
Packing group	II
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

National inventories

Substance is listed in the following national inventories:

Country	National inventories	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)

n-Heptane ≥99 %, for synthesis

article number: **8654**

Legend

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
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

16.1 Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.1	Remarks: For full text of Hazard- and EU Hazard-statements: see SECTION 16.		yes
2.2		Pictograms: change in the listing (table)	yes
2.2		Precautionary statements - prevention: change in the listing (table)	yes
2.2		Precautionary statements - response: 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
8.1		• human health values: change in the listing (table)	yes
14.3	Transport hazard class(es)	Transport hazard class(es): class 3 hazard - flammable liquids	yes
14.8	Particulars in the transport document: UN1206, HEPTANES, (heptane), 3, II, (D/E), environmentally hazardous	Particulars in the transport document: UN1206, HEPTANES, 3, II, (D/E), environmentally hazardous	yes
14.8	Particulars in the shipper's declaration: UN1206, HEPTANES, (heptane), 3, II, -4°C c.c., MARINE POLLUTANT	Particulars in the shipper's declaration: UN1206, HEPTANES, 3, II, -4°C c.c., MARINE POLLUTANT	yes
14.8	Marine pollutant: yes (hazardous to the aquatic environment)	Marine pollutant: yes (P) (hazardous to the aquatic environment)	yes
14.8		• International Civil Aviation Organization (ICAO-IATA/DGR)	yes
14.8		UN number: 1206	yes
14.8		Proper shipping name: Heptanes	yes
14.8		Particulars in the shipper's declaration: UN1206, Heptanes, 3, II	yes
14.8		Class: 3	yes
14.8		Environmental hazards: yes (hazardous to the aquatic environment)	yes

n-Heptane ≥99 %, for synthesis

article number: 8654

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
14.8		Packing group: II	yes
14.8		Danger label(s): 3	yes
14.8		Danger label(s): change in the listing (table)	yes
14.8		Excepted quantities (EQ): E2	yes
14.8		Limited quantities (LQ): 1 L	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland 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)
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DGR	Dangerous Goods Regulations (see IATA/DGR)
DMEL	Derived Minimal Effect Level
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
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
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
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
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
NOEC	No Observed Effect Concentration

Safety data sheet

Safe Work Australia - Code of Practice



n-Heptane ≥99 %, for synthesis

article number: 8654

Abbr.	Descriptions of used abbreviations
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
ppm	parts per million
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
TWA	time-weighted average
vPvB	very Persistent and very Bioaccumulative
WES	Safe Work Australia: Workplace exposure standards for airborne conatminants

Key literature references and sources for data

- UN Recommendations on the Transport of Dangerous Good
- Dangerous Goods Regulations (DGR) for the air transport (IATA)
- International Maritime Dangerous Goods Code (IMDG)

List of relevant phrases (code and full text as stated in chapter 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

Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.