

Heptane-(n) , LC-MS grade

Revision: 19.09.2025

Product code: AC11.00747

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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**

Heptane-(n) , LC-MS grade

Substance name: heptane
REACH Registration Number: 01-2119457603-38-XXXX
CAS No: 142-82-5
Index No: 601-008-00-2
EC No: 205-563-8

1.2. Relevant identified uses of the substance or mixture and uses advised against**Use of the substance/mixture**

Reagents and laboratory chemicals
Only for laboratory and analysis purposes.

Uses advised against

Do not use for private purposes (household).

1.3. Details of the supplier of the safety data sheet**Details of the supplier of the safety data sheet**

Company name: AnalytiChem Services, Unipessoal, Lda
Street: Rua de Júlio Dinis 676 7º
Place: N-4050-320 Porto
Telephone: +351 226002917
E-mail: info@analytichem.com
Contact person: SDS service department
E-mail: SDS@analytichem.com
Internet: www.analytichem.com
Responsible Department: SDS service department

Supplier or manufacturer details

Company name: AnalytiChem Belgium NV
Street: Industriezone "De Arend" 2
Place: B-8210 Zedelgem
Telephone: +32 50 28 83 20
E-mail: info.be@analytichem.com
Contact person: SDS service department
E-mail: SDS@analytichem.com
Responsible Department: AnalytiChem:
EU-Belgium: AnalytiChem Belgium, Industriezone "De Arend" 2, 8210 Zedelgem, Belgium, +32 50 28 83 20
EU-Germany: AnalytiChem Germany, Stempelstrasse 6, 47167 Duisburg, Germany, +49 203 51 94 – 200
EU-Netherlands: AnalytiChem Netherlands, Communicatieweg 7, 3641 SG Mijdrecht, The Netherlands, +31 297 286848
UK: AnalytiChem UK, Unit 7 Launton Business Center, Murdock Road, Bicester, OX26 4XB, England, +44 1869 355 500
USA: AnalytiChem USA, 227 China Road, Winslow, Maine, 04901, United States, +1 800-244-8378
Canada: AnalytiChem Canada, 21800 Clark Graham Avenue, Baie d'Urfe, H9X 4B6, Canada, +1 514-457-0701
Australia: ORE Research & Exploration Pty Ltd, 37A Hosie Street, Bayswater North, 3153, Australia, +61 3 9729 0333

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1.4. Emergency telephone number: +44 20 3807 3798 (CHEMTREC)

Further Information

No data available

SECTION 2: Hazards identification**2.1. Classification of the substance or mixture****Regulation (EC) No 1272/2008**

Flam. Liq. 2; H225
Skin Irrit. 2; H315
STOT SE 3; H336
Asp. Tox. 1; H304
Aquatic Acute 1; H400
Aquatic Chronic 1; H410

Full text of hazard statements: see SECTION 16.

2.2. Label elements**Regulation (EC) No 1272/2008****Signal word:** Danger**Pictograms:****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.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P273 Avoid release to the environment.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.
P331 Do NOT induce vomiting.
P391 Collect spillage.
P403+P235 Store in a well-ventilated place. Keep cool.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients**3.1. Substances**

Sum formula: C₇H₁₆
Molecular weight: 100.21 g/mol

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Relevant ingredients

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
142-82-5	heptane			100 %
	205-563-8	601-008-00-2	01-2119457603-38-XXXX	
	Flam. Liq. 2, Skin Irrit. 2, STOT SE 3, Asp. Tox. 1, Aquatic Acute 1, Aquatic Chronic 1; H225 H315 H336 H304 H400 H410			

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
	Specific Conc. Limits, M-factors and ATE		
142-82-5	205-563-8	heptane	100 %
	inhalation: LC50 = > 29,29 mg/l (vapours); dermal: LD50 = > 2000 mg/kg; oral: LD50 = > 5000 mg/kg		

Further Information

No data available

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

Remove contaminated, saturated clothing immediately.

After inhalation

Provide fresh air.

Call a physician immediately.

After contact with skin

Wash immediately with: Water

Take off immediately all contaminated clothing and wash it before reuse.

After contact with eyes

After contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately.

Remove contact lenses, if present and easy to do. Continue rinsing.

Protect uninjured eye.

After ingestion

Observe risk of aspiration if vomiting occurs.

Call a physician immediately.

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

Narcotic effects

May cause drowsiness or dizziness.

Has degreasing effect on the skin.

Pulmonary oedema

Pneumonia

4.3. Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1. Extinguishing media

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Suitable extinguishing media

Carbon dioxide (CO₂)
Foam
Extinguishing powder

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

Combustible liquids
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 dioxide
Carbon monoxide
Beware of reignition.

5.3. Advice for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing.

Additional information

Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.
Move undamaged containers from immediate hazard area if it can be done safely.
Use water spray jet to protect personnel and to cool endangered containers.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General advice

Vapours can form explosive mixtures with air. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

For non-emergency personnel

Provide adequate ventilation.
Use personal protection equipment.
Avoid contact with skin, eyes and clothes.
Remove persons to safety.
To follow: Emergency procedures
Do not breathe mist/vapours/spray.

For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

6.2. Environmental precautions

Do not allow to enter into surface water or drains.
Explosion risk.

6.3. Methods and material for containment and cleaning up

For containment

Cover drains.
Prevent spread over a wide area (e.g. by containment or oil barriers).
Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).
Collect in closed and suitable containers for disposal.

For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

Other information

Provide adequate ventilation.
Do not breathe mist/vapours/spray.

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Wear breathing apparatus if exposed to vapours/dusts/aerosols.

6.4. Reference to other sections

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13

SECTION 7: Handling and storage**7.1. Precautions for safe handling****Advice on safe handling**

Read label before use.

Handle and open container with care.

Use personal protection equipment.

Avoid contact with skin, eyes and clothes.

Do not breathe dust/fume/gas/mist/vapours/spray.

Provide adequate ventilation.

Use extractor hood (laboratory).

Avoid: aerosol or mist formation

Advice on protection against fire and explosion

Take precautionary measures against static discharges.

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

This material can be ignited by heat, sparks, flames, or other sources of ignition (e.g., static electricity, pilot lights, mechanical/electrical equipment, and electronic devices such as cell phones, computers, calculators, and pagers which have not been certified as intrinsically safe).

Advice on general occupational hygiene

Keep away from: Food and feedingstuffs

When using do not eat, drink, smoke, sniff.

Provide eye shower and label its location conspicuously

Further information on handling

Draw up and observe skin protection programme.

Wash hands and face before breaks and after work and take a shower if necessary.

Take off immediately all contaminated clothing and wash it before reuse.

7.2. Conditions for safe storage, including any incompatibilities**Requirements for storage rooms and vessels**

Keep container tightly closed.

Protect against: Radiant heat.

Keep away from sources of ignition - No smoking.

Hints on joint storage

National regulations

Further information on storage conditions

Store in a dry place.

Store in a well-ventilated place.

7.3. Specific end use(s)

Reagents and laboratory chemicals

SECTION 8: Exposure controls/personal protection**8.1. Control parameters**

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Exposure limits (EH40)

CAS No	Substance	ppm	mg/m ³	fibres/ml	Category	Origin
142-82-5	n-Heptane	500	2085		TWA (8 h)	WEL

DNEL/DMEL values

CAS No	Substance	Exposure route	Effect	Value
142-82-5	heptane			
Worker DNEL, long-term		inhalation	systemic	2085 mg/m ³
Worker DNEL, long-term		dermal	systemic	300 mg/kg bw/day
Consumer DNEL, long-term		inhalation	systemic	447 mg/m ³
Consumer DNEL, long-term		dermal	systemic	149 mg/kg bw/day
Consumer DNEL, long-term		oral	systemic	149 mg/kg bw/day

Additional advice on limit values

Observe in addition any national regulations!

8.2. Exposure controls

Appropriate engineering controls

Provide adequate ventilation as well as local exhaust at critical locations.

If technical exhaust or ventilation measures are not possible or insufficient, respiratory protection must be worn.

Individual protection measures, such as personal protective equipment

Eye/face protection

goggles

Face protection umbrella

Hand protection

Tested protective gloves must be worn

The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances.

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.

Skin protection

Wear suitable protective clothing.

When handling with chemical substances, protective clothing with CE-labels including the four control digits must be worn.

Take off immediately all contaminated clothing and wash it before reuse.

Respiratory protection

Wear breathing apparatus if exposed to vapours/dusts/aerosols.

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Thermal hazards

No data available

Environmental exposure controls

Do not allow to enter into surface water or drains.

Explosion risk.

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SECTION 9: Physical and chemical properties**9.1. Information on basic physical and chemical properties**

Physical state:	Liquid
Colour:	colourless
Odour:	like: Hydrocarbons
Odour threshold:	No data available
Melting point/freezing point:	-91 °C
Boiling point or initial boiling point and boiling range:	98.2-98.4 °C
Flammability:	No data available
Lower explosion limits:	1.1 vol. %
Upper explosion limits:	7 vol. %
Flash point:	-4 °C
Auto-ignition temperature:	223 °C
Decomposition temperature:	No data available
pH-Value:	No data available
Viscosity / kinematic: (at 20 °C)	0.64 mm²/s
Water solubility:	practically insoluble
Solubility in other solvents	
No data available	
Dissolution rate:	No data available
Partition coefficient n-octanol/water:	No data available
Dispersion stability:	No data available
Vapour pressure:	48 hPa
(at 20 °C)	
Vapour pressure:	No data available
Density (at 15 °C):	0.68 g/cm³
Relative density:	No data available
Bulk density:	No data available
Relative vapour density:	No data available
Particle characteristics:	No data available

9.2. Other information**Information with regard to physical hazard classes****Explosive properties**

Vapours can form explosive mixtures with air.

Sustained combustibility:

No data available

Self-ignition temperature

Solid:

No data available

Gas:

No data available

Oxidizing properties

No data available

Other safety characteristics**Evaporation rate:**

No data available

Solvent separation test:

No data available

Solvent content:

100%

Solid content:

0%

Sublimation point:

No data available

Softening point:

No data available

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Pour point: No data available
No data available:
Viscosity / dynamic: No data available
Flow time: No data available

Further Information

No data available

SECTION 10: Stability and reactivity**10.1. Reactivity**

Vapours can form explosive mixtures with air.

10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

10.3. Possibility of hazardous reactions

Oxidising agent, strong,

10.4. Conditions to avoid

Radiant heat.

10.5. Incompatible materialsRubber articles
Plastic articles**10.6. Hazardous decomposition products**

In case of fire may be liberated:

SECTION 5: Firefighting measures

Further information

No data available

SECTION 11: Toxicological information**11.1. Information on hazard classes****Acute toxicity**

Based on available data, the classification criteria are not met.

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
142-82-5	heptane				
	oral	LD50 > 5000 mg/kg	Rat	Study report (1982)	OECD Guideline 401
	dermal	LD50 > 2000 mg/kg	Rabbit	Study report (1982)	OECD Guideline 402
	inhalation (4 h) vapour	LC50 > 29,29 mg/l	Rat	Study report (1982)	OECD Guideline 403

Irritation and corrosivity

Skin corrosion/irritation: Causes skin irritation.

Serious eye damage/eye irritation: Based on available data, the classification criteria are not met.

Sensitising effects

Based on available data, the classification criteria are not met.

Carcinogenic/mutagenic/toxic effects for reproduction

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Germ cell mutagenicity: Based on available data, the classification criteria are not met.

Carcinogenicity: Based on available data, the classification criteria are not met.

Reproductive toxicity: Based on available data, the classification criteria are not met.

STOT-single exposure

May cause drowsiness or dizziness. (heptane)

STOT-repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

May be fatal if swallowed and enters airways.

Information on likely routes of exposure

No data available

Specific effects in experiment on an animal

No data available

Additional information on tests

No data available

Practical experience

No data available

11.2. Information on other hazards**Endocrine disrupting properties**

This substance does not have endocrine disrupting properties with respect to non-target organisms.

Other information

Narcotic effects

May cause drowsiness or dizziness.

Has degreasing effect on the skin.

Pulmonary oedema

Pneumonia

Further information

No data available

SECTION 12: Ecological information**12.1. Toxicity**

Very toxic to aquatic life.

Very toxic to aquatic life with long lasting effects.

CAS No	Chemical name						
	Aquatic toxicity	Dose		[h] [d]	Species	Source	Method
142-82-5	heptane						
	Acute algae toxicity	ErC50 mg/l	4,338	72 h	Pseudokirchneriella subcapitata	CONCAWE, Brussels, Belgium (2010)	The aquatic toxicity was estimated by a
	Acute crustacea toxicity	EC50	1,5 mg/l	48 h	Daphnia magna	Study report (1987)	other: As described in: The evaluation o
	Fish toxicity	NOEC mg/l	1,284	28 d	Oncorhynchus mykiss	CONCAWE, Brussels, Belgium (2010)	The aquatic toxicity was estimated by a
	Crustacea toxicity	NOEC	1 mg/l	21 d	Daphnia magna	SIDS Initial Assessment Report For SIAM	OECD Guideline 211

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12.2. Persistence and degradability

Readily biodegradable (according to OECD criteria).
(70% / 10d aerob)

12.3. Bioaccumulative potential**Partition coefficient n-octanol/water**

CAS No	Chemical name	Log Pow
142-82-5	heptane	4,5

BCF

CAS No	Chemical name	BCF	Species	Source
142-82-5	heptane	552	calculated	Other company data (

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of UK REACH.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

12.7. Other adverse effects

Discharge into the environment must be avoided.

Further information

Do not allow to enter into surface water or drains.

SECTION 13: Disposal considerations**13.1. Waste treatment methods****Disposal recommendations**

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.
Send to a physico-chemical treatment facility under observation of official regulations.
Do not allow to enter into surface water or drains.

Contaminated packaging

Handle contaminated packages in the same way as the substance itself.

SECTION 14: Transport information**Land transport (ADR/RID)**

14.1. UN number or ID number:	UN 1206
14.2. UN proper shipping name:	HEPTANES
14.3. Transport hazard class(es):	3
14.4. Packing group:	II
Hazard label:	3
Classification code:	F1
Limited quantity:	1 L
Excepted quantity:	E2
Transport category:	2
Hazard No:	33
Tunnel restriction code:	D/E

Inland waterways transport (ADN)

14.1. UN number or ID number:	UN 1206
14.2. UN proper shipping name:	HEPTANES
14.3. Transport hazard class(es):	3

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14.4. Packing group:

Hazard label: II
Classification code: 3
Limited quantity: F1
Excepted quantity: 1 L
Excepted quantity: E2

Marine transport (IMDG)

14.1. UN number or ID number: UN 1206
14.2. UN proper shipping name: HEPTANES
14.3. Transport hazard class(es): 3
14.4. Packing group: II
Hazard label: 3
Marine pollutant: P
Special Provisions: -
Limited quantity: 1 L
Excepted quantity: E2
EmS: F-E, S-D

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number: UN 1206
14.2. UN proper shipping name: HEPTANES
14.3. Transport hazard class(es): 3
14.4. Packing group: II
Hazard label: 3
Limited quantity Passenger: 1 L
Passenger LQ: Y341
Excepted quantity: E2
IATA-packing instructions - Passenger: 353
IATA-max. quantity - Passenger: 5 L
IATA-packing instructions - Cargo: 364
IATA-max. quantity - Cargo: 60 L

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: Yes
Danger releasing substance: heptane; n-heptane

14.6. Special precautions for user

No dangerous good in sense of this transport regulation.

14.7. Maritime transport in bulk according to IMO instruments

No dangerous good in sense of this transport regulation.

SECTION 15: Regulatory information**15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture****EU regulatory information**

Restrictions on use (REACH, annex XVII):

Entry 3, Entry 40, Entry 75

Information according to Directive 2012/18/EU (SEVESO III): E1 Hazardous to the Aquatic Environment

Additional information: P5c

Additional information

Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC).

National regulatory information

Water hazard class (D): 2 - obviously hazardous to water

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SECTION 16: Other information**Abbreviations and acronyms**

Flam. Liq. 2: Flammable liquids, hazard category 2

Asp. Tox. 1: Aspiration hazard, hazard category 1

Skin Irrit. 2: Skin irritation, hazard category 2

STOT SE 3: Specific target organ toxicity - single exposure, hazard category 3

Aquatic Acute 1: Hazardous to the aquatic environment, hazard category: Acute 1

Aquatic Chronic 1: Hazardous to the aquatic environment, long-term hazard category: Chronic 1

Relevant H and EUH statements (number and full 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.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

Further Information

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights.

The receiver of our product is singularly responsible for adhering to existing laws and regulations.