

Chemical Safety Data Sheet MSDS / SDS

Heptane

Revision Date:2026-01-17 Revision Number:1

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

Product identifier

Product name : Heptane
CBnumber : CB0426554
CAS : 142-82-5
EINECS Number : 205-563-8
Synonyms : Heptane,n-heptane

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P501 Dispose of contents/container to.....

P405 Store locked up.

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

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

P391 Collect spillage. Hazardous to the aquatic environment

P370+P378 In case of fire: Use ... for extinction.

P331 Do NOT induce vomiting.

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

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P273 Avoid release to the environment.

P271 Use only outdoors or in a well-ventilated area.

P264 Wash skin thoroughly after handling.

P264 Wash hands thoroughly after handling.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P240 Ground/bond container and receiving equipment.

P233 Keep container tightly closed.

P223 Keep away from any possible contact with water, because of violent reaction and possible flash fire.

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

Hazard statements

H410 Very toxic to aquatic life with long lasting effects

H400 Very toxic to aquatic life

H336 May cause drowsiness or dizziness

H335 May cause respiratory irritation

H333 May be harmful if inhaled

H320 Causes eye irritation

H319 Causes serious eye irritation

H315 Causes skin irritation

H304 May be fatal if swallowed and enters airways

H260 In contact with water releases flammable gases which may ignite spontaneously

H225 Highly Flammable liquid and vapour

SECTION 3: Composition/information on ingredients

Substance

Product name	: Heptane
Synonyms	: Heptane,n-heptane
CAS	: 142-82-5
EC number	: 205-563-8
MF	: C ₇ H ₁₆
MW	: 100.2

SECTION 4: First aid measures

Description of first aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

If swallowed

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) Foam Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture

Carbon oxides

Flash back possible over considerable distance. Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire. Forms explosive mixtures with air at ambient temperatures.

Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion. Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

NFPA 704

■ HEALTH 1 Exposure would cause irritation with only minor residual injury (e.g. [acetone](#), sodium bromate, potassium chloride)

Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature

■ FIRE 3 conditions . Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, [acetone](#))

■ REACT

□ SPEC.

□ HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

Environmental precautions

Do not let product enter drains. Risk of explosion.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g.

Chemizorb?). Dispose of properly. Clean up affected area.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Advice on safe handling

Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Store under inert gas.

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,4 mm Break through time: 480 min

Material tested: Camatril? (KCL 730 / Aldrich Z677442, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,2 mm Break through time: 60 min

Material tested: Dermatril? P (KCL 743 / Aldrich Z677388, Size M)

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

Exposure limits

NIOSH REL: TWA 85 ppm (350 mg/m³), 15-min ceiling 440 ppm (1,800 mg/m³), IDLH 750 ppm; OSHA PEL: TWA 500 ppm (2,000 mg/m³); ACGIH TLV: TWA 400 ppm, STEL 500 ppm (adopted).

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	liquid
Odour	No data available
Odour Threshold	0.67ppm
pH	No data available
Melting point/freezing point	Melting point/range: -91 °C
Initial boiling point and boiling range	98 °C
Flash point	-4 °C - c.c.
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 7 %(V) Lower explosion limit: 1,1 %(V)
Vapour pressure	111 hPa at 37,7 °C 53,3 hPa at 20,0 °C
Vapour density	3.5 (vs air)
Relative density	0.684 (20/4 °C)
Water solubility	insoluble
Partition coefficient: n-octanol/water	log Pow: >3 - Bioaccumulation is not expected.
Autoignition temperature	223,0 °C
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: 0,64 mm ² /s at 20 °C Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available
Henry's Law Constant	0.901, 1.195, and 1.905(atm·m ³ /mol) at 26.0, 35.8, and 45.0 °C, respectively (dynamic headspace, Hansen et al., 1995)
λmax	λ: 200 nm Amax: ≤1.0 λ: 225 nm Amax: ≤0.10 λ: 250 nm Amax: ≤0.01 λ: 300-400 nm Amax: ≤0.005

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

Vapors may form explosive mixture with air.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapours with:

Strong oxidizing agents phosphorus

in the presence of:

Chlorine

Conditions to avoid

Warming.

Incompatible materials

rubber, various plastics

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - > 5.000 mg/kg

(OECD Test Guideline 401)

Remarks: (in analogy to similar compounds)

The value is given in analogy to the following substances: isooctane LC50 Inhalation - Rat - male and female - 4 h - > 29,29 mg/l (OECD Test Guideline 403)

LD50 Dermal - Rabbit - male and female - > 2.000 mg/kg (OECD Test Guideline 402)

Remarks: The value is given in analogy to the following substances: isooctane

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h (OECD Test Guideline 404)

Remarks: The value is given in analogy to the following substances: isooctane Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation (OECD Test Guideline 405)

Remarks: The value is given in analogy to the following substances: isooctane

Respiratory or skin sensitization

(OECD Test Guideline 406) Remarks:

Test system: Escherichia coli/Salmonella typhimurium Metabolic activation: with and without metabolic activation Method: OECD Test Guideline

Result: negative

Test Type: Chromosome aberration test in vitro Test system: rat hepatocytes

Method: OECD Test Guideline 473 Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

May be fatal if swallowed and enters airways.

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

Toxicity

LC (2 hr in air) in mice: 75 mg/l (Lazarew)

SECTION 12: Ecological information

Toxicity

Toxicity to daphnia and other aquatic invertebrates

static test EC50 - Daphnia magna (Water flea) - 1,50 mg/l - 48 h Remarks: (ECHA)

Persistence and degradability

Biodegradability aerobic - Exposure time 10 d

Result: 70 % - Readily biodegradable. Remarks: (ECHA)

Biochemical Oxygen Demand (BOD)

Theoretical oxygen demand

1.920 mg/g Remarks: (IUCIID)

3.500 mg/g Remarks: (Lit.)

Ratio BOD/ThBOD 55 %

Remarks: (Lit.)

Bioaccumulative potential

Indication of bioaccumulation.

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and

very bioaccumulative (vPvB) at levels of 0.1% or higher.

Toxics Screening Level

The initial threshold screening level for heptane is 3500 µg/m³ based on an 8-hour averaging time.

Other adverse effects

Additional ecological information

Do not empty into drains.

Avoid release to the environment.

SECTION 13: Disposal considerations

Waste treatment methods

Incompatibilities

May form explosive mixture with air. Strong oxidizers may cause fire and explosions. Attacks some plastics, rubber and coatings. May accumulate static electric charges that can ignite its vapors.

Waste Disposal

Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. All federal, state, and local environmental regulations must be observed.

SECTION 14: Transport information

UN number

ADR/RID: 1206 IMDG: 1206

UN proper shipping name

ADR/RID: HEPTANES IMDG: HEPTANES IATA: Heptanes

Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

Packaging group

ADR/RID: II IMDG: II IATA: II

Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015: Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

Korea Existing Chemicals List (KECL): Listed. website: <http://ncis.nier.go.kr>

New Zealand Inventory of Chemicals (NZIoC): Listed. website: <https://www.epa.govt.nz/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS): Listed. website: <https://emb.gov.ph/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC): Listed. website: <https://www.mee.gov.cn/>

EC Inventory: Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS): Listed. website: <https://echa.europa.eu/>

Vietnam National Chemical Inventory: Listed. website: <https://chemicaldata.gov.vn/>

United States Toxic Substances Control Act (TSCA) Inventory: Listed. website: <https://www.epa.gov/>

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

[1] CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

[2] ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

[3] ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

[4] eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

[5] ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

[6] Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

[7] HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

[8] IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

[9] IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

[10] Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Other Information

The odour warning when the exposure limit value is exceeded is insufficient. The symptoms of chemical pneumonitis do not become manifest until a few hours or even days have passed.

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.