

SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.1
Creation Date: July 15, 2019
Revision Date: April 19, 2024

SECTION 1: Identification

1.1 GHS Product identifier

Product name N-Heptane

1.2 Other means of identification

Product number CCEM500635

Other names 1-HEPTANE; N-HEPTANE; ethyl-pentane

1.3 Recommended use of the chemical and restrictions on use

Identified uses For laboratory and Industrial use only.

Uses advised against no data available

1.4 Supplier's details

Company CATO Research Chemicals Inc.

Address 3/F,Building B,No.179 BASIGO, Guangpu Rd East,Huangpu Dist,Guangzhou

Telephone +86-20-81960175

1.5 Emergency phone number

Emergency phone number +86-20-81960175

Service hours 'Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Flammable liquids, Category 2

Skin irritation, Category 2

Aspiration hazard, Category 1

Specific target organ toxicity – single exposure, Category 3

Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

2.2 GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H225 Highly flammable liquid and vapour
H315 Causes skin irritation
H304 May be fatal if swallowed and enters airways
H336 May cause drowsiness or dizziness
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention	P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P233 Keep container tightly closed. P240 Ground and bond container and receiving equipment. P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment. P242 Use non-sparking tools. P243 Take action to prevent static discharges. P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/... P264 Wash ... thoroughly after handling. P261 Avoid breathing dust/fume/gas/mist/vapours/spray. P271 Use only outdoors or in a well-ventilated area. P273 Avoid release to the environment.
Response	P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower]. P370+P378 In case of fire: Use ... to extinguish. P302+P352 IF ON SKIN: Wash with plenty of water/... P321 Specific treatment (see ... on this label). P332+P317 If skin irritation occurs: Get medical help. P362+P364 Take off contaminated clothing and wash it before reuse. P301+P316 IF SWALLOWED: Get emergency medical help immediately. P331 Do NOT induce vomiting. P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing. P319 Get medical help if you feel unwell. P391 Collect spillage.
Storage	P403+P235 Store in a well-ventilated place. Keep cool. P405 Store locked up. P403+P233 Store in a well-ventilated place. Keep container tightly closed.
Disposal	P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
N-Heptane	Heptane	142-82-5	205-563-8	100%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Rinse and then wash skin with water and soap. Refer for medical attention if skin irritation occurs.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Give nothing to drink. Do NOT induce vomiting. Refer immediately for medical attention. See Notes.

4.2 Most important symptoms/effects, acute and delayed

VAPOR: Not irritating to eyes, nose or throat. If inhaled, will cause coughing or difficult breathing. LIQUID: Irritating to skin and eyes. If swallowed, will cause nausea or vomiting. (USCG, 1999)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Aliphatic hydrocarbons and related compounds

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

5.2 Specific hazards arising from the chemical

FLAMMABLE. Flashback along vapor trail may occur. Vapor may explode if ignited in an enclosed area. (USCG, 1999)

5.3 Special protective actions for fire-fighters

Use alcohol-resistant foam, dry powder, carbon dioxide, water spray. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Remove all ignition sources. Consult an expert! Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Do NOT wash away into sewer. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Carefully collect remainder. Then store and dispose of according to local regulations.

6.2 Environmental precautions

Remove all ignition sources. Consult an expert! Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Do NOT wash away into sewer. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Carefully collect remainder.

6.3 Methods and materials for containment and cleaning up

Collect leaking liquid in sealable containers... Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer. Personal protection: filter respirator for organic gases and vapors adapted to the airborne concentration of the substance.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

NO open flames, NO sparks and NO smoking. Closed system, ventilation, explosion-proof electrical equipment and lighting. Prevent build-up of electrostatic charges (e.g., by grounding). Do NOT use compressed air for filling, discharging, or handling. Use non-sparking handtools. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

7.2 Conditions for safe storage, including any incompatibilities

Fireproof. Separated from strong oxidants. Store in an area without drain or sewer access. Provision to contain effluent from fire extinguishing. Fireproof. Separated from strong oxidants. Store in an area without drain or sewer access.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

TLV: 400 ppm as TWA; 500 ppm as STEL. MAK: 2100 mg/m³, 500 ppm; peak limitation category: I(1); pregnancy risk group: D. EU-OEL: 2085 mg/m³, 500 ppm as TWA

Biological limit values

no data available

8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety goggles in combination with breathing protection.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	Liquid. Liquid.
Colour	Colorless liquid
Odour	Gasoline-like odor
Melting point/freezing point	-91 °C
Boiling point or initial boiling point and boiling range	98.2 - 98.4 °C. Atm. press.:100 kPa. Remarks:Distillation range.
Flammability	Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F.
Lower and upper explosion limit/flammability limit	no data available
Flash point	-4 °C.
Auto-ignition temperature	204 °C.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	kinematic viscosity (in mm²/s) = 0.641. Temperature:20°C.
Solubility	Insoluble in water
Partition coefficient n-octanol/water	log Pow = 4.5.
Vapour pressure	6.09 kPa. Temperature:25 °C.
Density and/or relative density	0.69 g/cm³. Temperature:15 °C.
Relative vapour density	3.5 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Reacts violently with strong oxidants. This generates fire and explosion hazard. Attacks many plastics.

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

Highly flammable liquid and vapor.The vapour is heavier than air and may travel along the ground; distant ignition possible. As a result of flow, agitation, etc., electrostatic charges can be generated.HEPTANE is incompatible with the following: Strong oxidizers (NIOSH, 2016).

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Violent reaction with phosphorous + chlorine.

10.6 Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 - rat (male/female) - > 5 000 mg/kg bw.
- Inhalation: LC50 - rat (male/female) - > 29.29 mg/L air (nominal).
- Dermal: LD50 - rabbit (male/female) - > 2 000 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

CLASSIFICATION: D; not classifiable as to human carcinogenicity. BASIS FOR CLASSIFICATION: No human data and no animal data available. HUMAN CARCINOGENICITY DATA: None. ANIMAL CARCINOGENICITY DATA: None.

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the skin. The vapour is irritating to the respiratory tract. If swallowed the substance easily enters the airways and could result in aspiration pneumonitis. The substance may cause effects on the central nervous system.

STOT-repeated exposure

The substance defats the skin, which may cause dryness or cracking.

Aspiration hazard

A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20°C.

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LL50 - *Oncorhynchus mykiss* (previous name: *Salmo gairdneri*) - 5.738 mg/L - 96 h.
- Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 1.5 mg/L - 48 h.
- Toxicity to algae: EL50 - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - 4.338 mg/L - 72 h.
- Toxicity to microorganisms: EL50 - *Tetrahymena pyriformis* - 22.6 mg/L - 48 h.

12.2 Persistence and degradability

AEROBIC: n-Heptane, present at 100 mg/L, reached 101% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test(1). In a study determining the primary aerobic biodegradation of biodiesel B20 fuel, the calculated half-life of n-heptane contained in the mixture was 2.3 days using unacclimated inocula from a rainwater detention pond(2). The theoretical oxygen demand of benzene acclimated activated sludge for n-heptane was 0.7, 4.3 and 23.4% after 6, 24, and 72 hr, respectively(3). One mg of n-heptane and 1 ml of a 1:10 suspension of Hudson-Collamer silt loam soil in mineral salts media were incubated in the dark at 25 deg C(4). Controls without n-heptane were used to determine the net oxygen consumed(4). The average theoretical biological oxygen demand of trials for n-heptane was 28, 63, 70 and 70% after 2, 5, 10 and 20 days, respectively(4). n-Heptane (5 ml) was completely degraded 4 days after it was added to a microcosm inoculated with soil from a gasoline contaminated site(5). At intervals of 6, 12 and 24 hr, endogenous respiration was greater than that of 3 preparations of n-heptane and activated sludge from differing aeration units of sewage treatment facilities(6). n-Heptane was degraded to approximately 17% of its initial concentration (unspecified) after 2 days and 100% after 25 days, respectively, in gasoline (400 mg/L) inoculated with activated aerobic sewage sludge (100 mg dry wt/L)(7).

12.3 Bioaccumulative potential

An estimated BCF of 550 was calculated in fish for n-heptane(SRC), using a log Kow of 4.66(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high(SRC), provided the compound is not metabolized by the organism(SRC).

12.4 Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of n-heptane can be estimated to be 240(SRC). According to a classification scheme(2), this estimated Koc value suggests that n-heptane is expected to have moderate mobility in soil.

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

14.1 UN Number

ADR/RID: UN1206 (For reference only, please check.) IMDG: UN1206 (For reference only, please check.) IATA: UN1206 (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: HEPTANES (For reference only, please check.) IMDG: HEPTANES (For reference only, please check.) IATA: HEPTANES (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.) IMDG: 3 (For reference only, please check.) IATA: 3 (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: II (For reference only, please check.) IMDG: II (For reference only, please check.) IATA: II (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: Yes

IMDG: Yes

IATA: Yes

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
Heptane	Heptane	142-82-5	205-563-8
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			Listed.
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Listed.

SECTION 16: Other information

Information on revision

Creation Date July 15, 2019

Revision Date April 19, 2024

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

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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.

Any questions regarding this SDS, Please send your inquiry to info@cato-chem.com

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