

SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.1
Creation Date: July 15, 2019
Revision Date: April 26, 2024

SECTION 1: Identification

1.1 GHS Product identifier

Product name N-Hexadecane

1.2 Other means of identification

Product number LCAD302331-TR
Other names -

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
2,2,4-trimethylpentane	2,2,4-trimethylpentane	540-84-1	208-759-1	100%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

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. Do NOT induce vomiting. Refer for medical attention.

4.2 Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: Inhalation or contact with material may irritate or burn skin and eyes. Fire may produce irritating, corrosive and/or toxic gases. Vapors may cause dizziness or suffocation. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

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

Absorption, Distribution and Excretion

Respiration is the most likely route by which 2,2,4-trimethylpentane is absorbed. Although it has not been determined, the respiratory uptake of 2,2,4-trimethylpentane is probably similar to that seen for n-octane. Oral absorption of (14)C-2,2,4-trimethylpentane has been reported ... to occur to the extent of 86% in male rats based on recovery of radioactivity in urine, expired organics, and expired (14)C-carbon dioxide. Dermal bioavailability has not been reported, but absorption of 2,2,4-trimethylpentane through the skin would be expected to be minor based on percutaneous results reported for n-heptane and n-octane. Oral gavage studies ... in male rats with (14)C-2,2,4-

trimethylpentane (0.5 mg/kg, single dose) revealed that the radioactivity is selectively distributed in the kidneys 72 hr after administration. It has been suggested that the renal retention of 2,2,4-trimethylpentane is related to the hydrocarbon-induced nephropathy observed specifically in male rats.

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: CAUTION: All these products have a very low flash point: Use of water spray when fighting fire may be inefficient. CAUTION: For mixtures containing alcohol or polar solvent, alcohol-resistant foam may be more effective. SMALL FIRE: Dry chemical, CO₂, water spray or regular foam. LARGE FIRE: Water spray, fog or regular foam. Do not use straight streams. Move containers from fire area if you can do it without risk. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. For massive fire, use unmanned hose holders or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2016)

5.2 Specific hazards arising from the chemical

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. Substance may be transported hot. For hybrid vehicles, ERG Guide 147 (lithium ion batteries) or ERG Guide 138 (sodium batteries) should also be consulted. If molten aluminum is involved, refer to ERG Guide 169. (ERG, 2016)

5.3 Special protective actions for fire-fighters

Use powder, AFFF, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water. Combat fire from a sheltered position.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Evacuate danger area! Personal protection: self-contained breathing apparatus. Remove all ignition sources. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

6.2 Environmental precautions

Evacuate danger area! Personal protection: self-contained breathing apparatus. Remove all ignition sources. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

6.3 Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

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. 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. Cool. Keep in a well-ventilated room.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

MAK: 470 mg/m³, 100 ppm; peak limitation category: II(2); pregnancy risk group: D

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.

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	MOBILE LIQUID
Odour	ODOR OF GASOLINE
Melting point/freezing point	-107 °C
Boiling point or initial boiling point and boiling range	99.2 °C. Atm. press.:100 kPa. Remarks:Distillation range.
Flammability	Highly flammable.
Lower and upper explosion limit/flammability limit	LOWER FLAMMABLE LIMIT: 1.1% BY VOLUME, UPPER FLAMMABLE LIMIT: 6.0% BY VOLUME
Flash point	-12 °C.
Auto-ignition temperature	418 °C.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	dynamic viscosity (in mPa s) = 0.5. Temperature:20°C.;dynamic viscosity (in mPa s) = 0.46. Temperature:25.0°C.;dynamic viscosity (in mPa s) = 0.38. Temperature:40°C.
Solubility	Insoluble in water
Partition coefficient n-octanol/water	log Pow = 4.08.
Vapour pressure	2.8 kPa. Temperature:20 °C.
Density and/or relative density	0.69 g/cm³. Temperature:15 °C.
Relative vapour density	3.9 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Heating may cause violent combustion or explosion. Reacts with strong oxidants.

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

Flammable, dangerous fire riskThe 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.Saturated aliphatic hydrocarbons, such as ISOCTANE, may be incompatible with strong oxidizing agents like nitric acid. Charring of the hydrocarbon may occur followed by ignition of unreacted hydrocarbon and other nearby combustibles. In other settings, aliphatic saturated hydrocarbons are mostly unreactive. They are not affected by aqueous solutions of acids, alkalis, most oxidizing agents, and most reducing agents.

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 - rat (male/female) - > 5 000 mg/kg bw.
- Inhalation: LC50 - rat (male/female) - > 33.52 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

no data available

Reproductive toxicity

No information is available on the reproductive or developmental effects of 2,2,4-trimethylpentane in humans or animals.

STOT-single exposure

The substance is irritating to the eyes, skin and respiratory tract. The substance may cause effects on the kidneys, liver and nervous system. If this liquid is swallowed, aspiration into the lungs may result in chemical pneumonitis.

STOT-repeated exposure

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

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50 - *Oncorhynchus mykiss* (previous name: *Salmo gairdneri*) - 0.11 mg/L - 96 h.
- Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 0.4 mg/L - 48 h.
- Toxicity to algae: EL50 - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - 2.943 mg/L - 72 h.
- Toxicity to microorganisms: EL50 - *Tetrahymena pyriformis* - 15.33 mg/L - 48 h.

12.2 Persistence and degradability

Branched octanes ... 2,2,4-trimethylpentane ... used as the sole carbon sources by a variety of microorganisms, such as *Pseudomonas fluorescens*, *Corynebacterium*, & *P. oleovorans*.

12.3 Bioaccumulative potential

Based upon a water solubility of 2.44 mg/L at 25 deg C(1), the log bioconcentration factor for iso-octane has been estimated to be 2.57 from a regression equation(2). This value indicates bioconcentration may be important in aquatic organism(SRC).

12.4 Mobility in soil

The adsorption of several hydrocarbons including iso-octane in five types of soil was studied by measuring the retention volumes(1). Hydrocarbon retention by dry soils increased with molecular weight and unsaturation and decreased with branching. The retention volume of iso-octane was found to be high, but the authors did not provide any Koc values. The log Koc for iso-octane in soil has been estimated to be 3.43 from the water solubility of the compound(4) and a regression equation(2). The average log Koc for this compound in sediments from a salt marsh, a pond and a river was 4.35. Therefore, iso-octane is expected to generally remain strongly adsorbed to soil and sediments(5,SRC).

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: UN1262 (For reference only, please check.) IMDG: UN1262 (For reference only, please check.) IATA: UN1262 (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: OCTANES (For reference only, please check.)

IMDG: OCTANES (For reference only, please check.)

IATA: OCTANES (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
2,2,4-trimethylpentane	2,2,4-trimethylpentane	540-84-1	208-759-1
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 26, 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/>

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

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