Chemical Safety Data Sheet MSDS / SDS

N-hexane SDS

Revision Date:2024-04-25 Revision Number:1

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

Product identifier

Product name: N-hexane

CAS: 110-54-3

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.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

Telephone: +91 9550333722

SECTION 2: Hazards identification

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
Specific target organ toxicity – repeated exposure, Category 2
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2
Reproductive toxicity, Category 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
H373 May cause damage to organs through prolonged or repeated exposure
H411 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.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P273 Avoid release to the environment.
P203 Obtain, read and follow all safety instructions before use.

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.
P318 IF exposed or concerned, get medical advice.

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.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	N-hexane
Common names and synonyms:	N-hexane
CAS number:	110-54-3
EC number:	203-777-6
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention .

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. Rest. Refer for medical attention .

Most important symptoms/effects, acute and delayed

INHALATION causes irritation of respiratory tract, cough, mild depression, cardiac arrhythmias. ASPIRATION causes severe lung irritation, coughing, pulmonary edema; excitement followed by depression. INGESTION causes nausea, vomiting, swelling of abdomen, headache, depression. (USCG, 1999)

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

Ingestion: Do not induce vomiting. Skin or eyes: Wipe off; wash skin with soap and water; wash eyes with copious amounts of water.

SECTION 5: Firefighting measures

Suitable extinguishing media

Stop discharge if possible. Keep people away. Shut off ignition sources and call fire department. Stay upwind and use water spray to "knock down" vapor. Isolate and remove discharged material. Notify local health and pollution control agencies.

Specific hazards arising from the chemical

Behavior in Fire: Vapors may explode (USCG, 1999)

Special protective actions for fire-fighters

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

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Consult an expert! Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Remove all ignition sources. Do NOT wash away into sewer. Do NOT let this chemical enter the environment. 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.

Environmental precautions

Consult an expert! Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Remove all ignition sources. Do NOT wash away into sewer. Do NOT let this chemical enter the environment. 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.

Methods and materials for containment and cleaning up

In the event of spillage, naked flames, sparks, and heat should be avoided; approved, efficient, protective clothing and respirators should be provided. Small-scale spillage should be absorbed on paper towels or sawdust; sand or earth can be used for larger spills. Fire-fighting foam can be used in large spillages to reduce evaporation. If possible, liquid spills should be recovered for recycling.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Closed system, ventilation, explosion-proof electrical equipment and lighting. 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.

Conditions for safe storage, including any incompatibilities

Fireproof. Separated from strong oxidants. Well closed.Drums should be stored in a well-ventilated area in fire-resistant containers. Metal containers should be electrically-grounded, when liquid is being transferred.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 50 ppm as TWA; (skin); BEI issued.MAK: 180 mg/m3, 50 ppm; peak limitation category: II(8); pregnancy risk group: C.EU-OEL: 72 mg/m3, 20 ppm as TWA

Biological limit values

no data available

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.

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

Eye/face protection

Wear safety goggles, face shield or eye protection 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:	N-hexane is a clear colorless liquids with a petroleum-like odor. Flash points -9°F. Less dense than water and insoluble in water. Vapors heavier than air. Used as a solvent, paint thinner, and chemical reaction medium.

Colour:	Liquid
Odour:	Gasoline-like odor
Melting point/freezing point:	-95°C(lit.)
Boiling point or initial boiling point and boiling range:	69°C(lit.)
Flammability:	Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F.
Lower and upper explosion limit/flammability limit:	Lower flammable limit: 1.1%, Upper flammable limit: 7.5% (by volume)
Flash point:	-26°C
Auto-ignition temperature:	453°F
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	3.26X10-4 Pa-s at 20 deg C
Solubility:	less than 1 mg/mL at 61.7° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Kow = 3.90
Vapour pressure:	120 mm Hg at 68° F ; 180 mm Hg at 77° F (NTP, 1992)
Density and/or relative density:	0.659g/mLat 25°C(lit.)
Relative vapour density:	~3 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

1100 ppm (Based on 10% of the lower explosion limit for safety considerations even though the relevant toxicological data indicated that irreversible health effects or impairment of escape existed only at higher concentrations.)
Reacts with strong oxidants. This generates fire and explosion hazard. Attacks some plastics, rubber and coatings.

Chemical stability

no data available

Possibility of hazardous reactions

Flammable. Flashback along vapor trail may occur.The vapour is heavier than air and may travel along the ground; distant ignition possible.HEXANE may be sensitive to light. It may also be sensitive to prolonged exposure to heat. This compound can react vigorously with oxidizing materials. This would include compounds such as liquid chlorine, concentrated O2, sodium hypochlorite and calcium hypochlorite. It is also incompatible with dinitrogen tetraoxide. It will attack some forms of plastics, rubber and coatings. (NTP, 1992).

Conditions to avoid

no data available

Incompatible materials

Forms explosive mixture with air. Contact with strong oxidizers may cause fire and explosions. contact with dinitrogen tetreoxide may explode at 28 deg C. Attacks some plastics, rubber and coatings. may accumulate static electrical charges, and may cause ignition of its vapor.

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Mouse oral 5000 mg/kg bw

Inhalation: LC50 Rat inhalation 48000 ppm/< 4 hr

Dermal: no data available

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

EPA-II

Reproductive toxicity

No information is available on the reproductive or developmental effects of hexane in humans. Testicular damage has been observed in male rats exposed to hexane via inhalation. Teratogenic effects were not observed in the offspring of rats chronically exposed via inhalation in several studies.

STOT-single exposure

The substance is irritating to the skin. If this liquid is swallowed, aspiration into the lungs may result in chemical pneumonitis. Exposure at high levels could cause lowering of consciousness.

STOT-repeated exposure

Repeated or prolonged contact with skin may cause dermatitis. The substance may have effects on the central nervous system and peripheral nervous system. This may result in polyneuropathy. Animal tests show that this substance possibly causes toxic effects upon human reproduction.

Aspiration hazard

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

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50; Species: Pimephales promelas (Fathead Minnow) age 31 days, length 20.4 mm, weight 0.123 g; Conditions: freshwater, flow through, 25.6 deg C, pH 7.4, hardness 44.7 mg/L CaCO3, alkalinity 43.9 mg/L CaCO3, dissolved oxygen 7.5 mg/L; Concentration: 2500 ug/L for 96 hr (95% confidence interval: 2100-2980 ug/L) /99+% purity

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water Flea) age 4-6 days, length 1.5 mm; Conditions: freshwater, static, 23 deg C, pH 6-7, dissolved oxygen 5-9 mg/L; Concentration: 45 mmol/cu m for 48 hr (95% confidence interval: 30-66 mmol/cu m); Effect: intoxication, immobilization /> or =97% purity formulation

Toxicity to algae: EC50; Species: Chlamydomonas angulosa (Green Algae) age 3-4 days, exponential growth phase 5x10+4 cells/mL; Conditions: static, 19 deg C, pH 6.5; Concentration: 94 mmol/cu m for 3 hr; Effect: physiology, photosynthesis /formulation

Toxicity to microorganisms: no data available

Persistence and degradability

The degradation of n-alkanes by microorganisms is similar to the degradation of fatty acids. The terminal methyl group is enzymatically oxidized by incorporation of molecular oxygen by a monooxygenase producing a primary alcohol with further oxidation to an acid group, although involvement of a dioxygenase is also postulated. Once the fatty acid is produced, it is degraded into 2-carbon units via the beta-oxidation pathway. ... Another pathway for n-alkane degradation that is encountered less often is the oxidation of both terminal carbons to form a dioic acid with subsequent beta-oxidation. Subterminal oxidation of the 2-carbon atom is seen mainly in C3-C6 alkanes, although it does occur in longer chain alkanes also. ... A dehydrogenation of the n-alkane may also occur yielding an alkene which is then converted to an alcohol, although there is little evidence for this theory. Some microorganisms have been shown to have both terminal and subterminal oxidation, each having very different rates of activity. The different chain lengths of n-alkanes are degraded to different extents . /In a study comparing/ ... growth on long an short chain alkanes by some bacteria ... the initial oxygenase had a broad specificity and would oxidize C1-C8 alkanes ... /but/ cells grown on C4-C8 alkanes did not oxidize the shorter chain alkanes to a significant extent. ... n-Alkanes

Bioaccumulative potential

An estimated BCF of 170 was calculated in fish for n-hexane(SRC), using a log Kow of 3.90(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).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of n-hexane can be estimated to be 130(SRC). According to a classification scheme(2), this estimated Koc value suggests that n-hexane is expected to have high mobility in soil.

Other adverse effects

no data available

SECTION 13: Disposal considerations

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

UN Number

ADR/RID: UN1208 (For reference only, please check.)
IMDG: UN1208 (For reference only, please check.)
IATA: UN1208 (For reference only, please check.)

UN Proper Shipping Name

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

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.)

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.)

Environmental hazards

ADR/RID: Yes
IMDG: Yes
IATA: Yes

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

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

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.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

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

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

Depending on the degree of exposure, periodic medical examination is suggested.