

Chemical Safety Data Sheet MSDS / SDS

HEXANES, MIXTURE OF ISOMERS, FOR SPECTROSCOPY, 95+%Revision Date:2023-12-07 Revision Number:1

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

Product name : HEXANES, MIXTURE OF ISOMERS, FOR SPECTROSCOPY, 95+%

CBnumber : CB9500790

CAS : 92112-69-1

EINECS Number : 295-570-2

Synonyms : Hexane, branched and linear,ISOHEXANE FOR ANALYSIS EMSURE

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 : 400-158-6606

SECTION 2: Hazards identification**Classification of the substance or mixture**

Skin irritation, Category 2

Skin sensitization, Category 1

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

Label elements**Pictogram(s)**

□□□□

Signal word : Danger

Hazard statement(s)

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

H361 Suspected of damaging fertility or the unborn child

H373 May cause damage to organs through prolonged or repeated exposure

H411 Toxic to aquatic life with long lasting effects

Precautionary statement(s)

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

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

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

P405 Store locked up.

Prevention

P264 Wash ... thoroughly after handling.

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

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

P272 Contaminated work clothing should not be allowed out of the workplace.

P273 Avoid release to the environment.

Response

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.

P333+P317 If skin irritation or rash occurs: Get medical help.

Storage

none

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

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: HEXANES, MIXTURE OF ISOMERS, FOR SPECTROSCOPY, 95+%
Synonyms	: Hexane, branched and linear,ISOHEXANE FOR ANALYSIS EMSURE
CAS	: 92112-69-1
EC number	: 295-570-2
MF	: C6H14
MW	: 86.1754

SECTION 4: First aid measures

Description of 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 and effects, both 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 any immediate medical attention and special treatment needed

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

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.

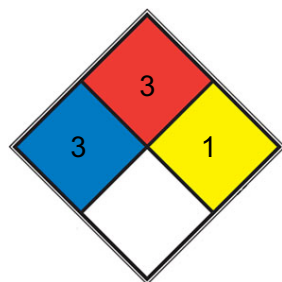
Specific Hazards Arising from the Chemical

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

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

NFPA 704



■ HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

■ FIRE 3 Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature 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 1 Normally stable, but can become unstable at elevated temperatures and pressures (e.g. [propene](#))

□ SPEC.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

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

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

Component	Hexane, branched and linear
CAS No.	92112-69-1
	Recommended Exposure Limit: 10 Hour Time-Weighted Average: 50 ppm (180 mg/cu m).

Biological limit values

no data available

Exposure 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

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Liquid, Mixture Of 5 Isomers
Colour	Colorless
Odour	Gasoline-like odor
Melting point/freezing point	-95°C
Boiling point or initial boiling point and boiling range	69°C
Flammability	Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F.
Lower and upper explosion limit/flammability limit	1.0-7.4%(V)
Flash point	-9.4° F (NTP, 1992)
Auto-ignition temperature	437° F (USCG, 1999)
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	160 - 190 hPa (20 °C)
Density and/or relative density	0.675g/cm ³
Relative vapour density	2.97 (NTP, 1992) (Relative to 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 tetroxide. 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 tetroxide 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

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

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 5x10⁴ 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: no data available

IMDG: no data available

IATA: no data available

UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

Transport hazard class(es)

ADR/RID: no data available

IMDG: no data available

IATA: no data available

Packing group, if applicable

ADR/RID: no data available

IMDG: no data available

IATA: no data available

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

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

Not Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

PICCS

Not Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Not Listed.

Korea Existing Chemicals List (KECL)

Not 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?pagelD=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/>

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