

## Chemical Safety Data Sheet MSDS / SDS

## N-HEXANE-D14

Revision Date:2023-11-29 Revision Number:1

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

## Product identifier

Product name : N-HEXANE-D14  
CBnumber : CB0250371  
CAS : 21666-38-6  
Synonyms : hexane-d14,N-HEXANE-D14, PACKAGED IN AMPULES, 99 ATOM% D, FOR NMR

## 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

## GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

## Precautionary statements

P405 Store locked up.  
P403+P235 Store in a well-ventilated place. Keep cool.  
P370+P378 In case of fire: Use ... for extinction.  
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.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

## Hazard statements

H411 Toxic to aquatic life with long lasting effects  
H401 Toxic to aquatic life

H373 May cause damage to organs through prolonged or repeated exposure

H361 Suspected of damaging fertility or the unborn child

H336 May cause drowsiness or dizziness

H315 Causes skin irritation

H304 May be fatal if swallowed and enters airways

H225 Highly Flammable liquid and vapour

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: N-HEXANE-D14
Synonyms	: hexane-d14,N-HEXANE-D14, PACKAGED IN AMPULES, 99 ATOM% D, FOR NMR
CAS	: 21666-38-6
MF	: C6D14
MW	: 100.26

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

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

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 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

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

## Special hazards arising from the substance or mixture

Carbon oxides

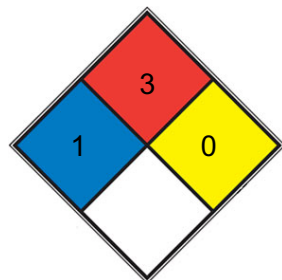
## Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

## Further information

Use water spray to cool unopened containers.

## 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 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

□ SPEC.

□ HAZ.

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## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition.

Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

### Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

### Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

### Reference to other sections

For disposal see section 13.

## SECTION 7: Handling and storage

### Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

### Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

### Specific end use(s)

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

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## SECTION 8: Exposure controls/personal protection

### control parameter

#### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

### Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

##### Eye/face protection

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

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

##### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance colorless clear, liquid

Odour No data available

Odour Threshold No data available

pH No data available

Melting point/freezing point -95 °C

Initial boiling point and boiling range 69 °C

Flash point -12 °C - closed cup

Evaporation rate No data available

Flammability (solid, gas) No data available

Upper/lower flammability or explosive limits 1.0-8.1%(V)

limits

Vapour pressure 132 mm Hg ( 20 °C)

Vapour density 3 (vs air)

Relative density 0,767 g/mL at 25 °C 0,767 g/cm<sup>3</sup> at 25 °C

Water solubility 0.0095g/l

Partition coefficient: n-octanol/water No data available

Autoignition temperature No data available

Decomposition temperature No data available

Viscosity No data available

Explosive properties No data available

Oxidizing properties No data available

### Other safety information

No data available

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## SECTION 10: Stability and reactivity

### Reactivity

No data available

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

No data available

### Conditions to avoid

Heat, flames and sparks.

## Incompatible materials

No data available

## Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides Other decomposition products - No data available

In the event of fire: see section 5

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# SECTION 11: Toxicological information

## Information on toxicological effects

### Acute toxicity

No data available

### Skin corrosion/irritation

No data available

### Serious eye damage/eye irritation Respiratory or skin sensitization

No data available

### Germ cell mutagenicity Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

### Reproductive toxicity

Suspected human reproductive toxicant

### Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

### Specific target organ toxicity - repeated exposure

Inhalation - May cause damage to organs through prolonged or repeated exposure.

### Aspiration hazard

The substance or mixture is known to cause human aspiration toxicity hazards or has to be regarded as if it causes a human aspiration toxicity hazard.

### Additional Information

RTECS: Not available

Central nervous system depression, Lung irritation, chest pain, pulmonary edema, giddiness, slowed reaction time, slurred speech, Headache, Dizziness, Drowsiness, Unconsciousness, Neurotoxic effects., Prolonged or repeated contact with skin may cause:, defatting, Dermatitis, Contact with eyes can cause:, Redness, Blurred vision, Provokes tears., Effects due to ingestion may include:, Gastrointestinal discomfort

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# SECTION 12: Ecological information

## Toxicity

No data available

## Persistence and degradability

No data available

### **Bioaccumulative potential**

No data available

### **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.

### **Other adverse effects**

Toxic to aquatic life.

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## **SECTION 13: Disposal considerations**

### **Waste treatment methods**

#### **Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

#### **Contaminated packaging**

Dispose of as unused product.

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## **SECTION 14: Transport information**

### **UN number**

ADR/RID: 1208 IMDG: 1208

### **UN proper shipping name**

ADR/RID: HEXANES

### **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

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## 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:Not Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

EC Inventory:Not Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

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## SECTION 16: Other information

### Abbreviations and acronyms

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

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

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

STEL: Short term exposure limit

TWA: Time Weighted Average

### 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](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/>



**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.