

## Chemical Safety Data Sheet MSDS / SDS

**HEXYL ISOTHIOCYANATE**

Revision Date:2025-02-01 Revision Number:1

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

Product name : HEXYL ISOTHIOCYANATE  
CBnumber : CB3221688  
CAS : 4404-45-9  
EINECS Number : 224-549-2  
Synonyms : Hexyl isothiocyanate,Hexane, 1-isothiocyanato-

**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.

P311 Call a POISON CENTER or doctor/physician.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.

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.

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

**Hazard statements**

H335 May cause respiratory irritation

H331 Toxic if inhaled  
H319 Causes serious eye irritation  
H318 Causes serious eye damage  
H315 Causes skin irritation  
H314 Causes severe skin burns and eye damage  
H312 Harmful in contact with skin  
H311 Toxic in contact with skin  
H302 Harmful if swallowed  
H301 Toxic if swallowed  
H227 Combustible liquid

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## SECTION 3: Composition/information on ingredients

### Substance

Product name : HEXYL ISOTHIOCYANATE  
Synonyms : Hexyl isothiocyanate, Hexane, 1-isothiocyanato-  
CAS : 4404-45-9  
EC number : 224-549-2  
MF : C7H13NS  
MW : 143.25

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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. Take victim immediately to hospital. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### 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.

#### Unsuitable extinguishing media

Do NOT use water jet.

### Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NOx) Sulfur oxides Combustible.

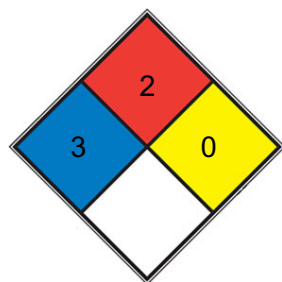
### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### Further information

Use water spray to cool unopened containers.

### 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 2** Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

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

**SPEC.**

**HAZ.**

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. 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.

### **Methods and materials for containment and cleaning up**

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.

### **Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **Precautions for safe handling**

#### **Advice on safe handling**

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

#### **Advice on protection against fire and explosion**

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

#### **Hygiene measures**

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

For precautions see section 2.2.

### **Conditions for safe storage, including any incompatibilities**

#### **Storage conditions**

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 in cool place.

#### **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**

#### **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, 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 ABEK (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.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	light yellow clear, liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	83 °C
Initial boiling point and boiling range	136 - 138 °C at 130 hPa - lit.
Flash point	91 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	No data available
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: 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

Strong oxidizing agents  
Strong bases

### Hazardous decomposition products

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

LC50 Inhalation - 4 h - 3 mg/l (Acute toxicity estimate) LD50 Dermal - 300 mg/kg

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

No data available

#### 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

No data available

#### Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

#### Specific target organ toxicity - repeated exposure

No data available

**Aspiration hazard**

No data available

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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**

No data available

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## SECTION 13: Disposal considerations

**Waste treatment methods**

**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

**Contaminated packaging**

Dispose of as unused product.

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## SECTION 14: Transport information

**UN number**

ADR/RID: - IMDG: - IATA: 3334

## UN proper shipping name

ADR/RID: Not dangerous goods IMDG: Not dangerous goods

IATA: Aviation regulated liquid, n.o.s.

14.3 Transport hazard class(es)

ADR/RID: - IMDG: - IATA: 9

Packaging group

14.4 ADR/RID: - IMDG: - IATA: III

Environmental hazards

14.5 ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

14.6 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

EC Inventory:Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

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

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

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

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

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

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

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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.