

Chemical Safety Data Sheet MSDS / SDS

HEXYL ISOTHIOCYANATE

Revision Date:2026-05-31 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 : 010-86108875

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

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

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

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.

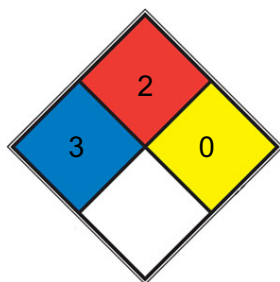
Advice for firefighters

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, [N2](#))

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.

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

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.

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

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

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

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

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.

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

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

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/>

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

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

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

EC Inventory:Listed.

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
- 【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:

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