

# Chemical Safety Data Sheet MSDS / SDS

## ISOTHIOCYANIC ACID 4-PENTEN-1-YL ESTER

Revision Date:2024-07-27 Revision Number:1

---

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

#### Product identifier

Product name : ISOTHIOCYANIC ACID 4-PENTEN-1-YL ESTER  
CBnumber : CB9176636  
CAS : 18060-79-2  
Synonyms : 4-PENTEN-1-YL ISOTHIOCYANATE,5-Isothiocyanato-1-pentene

#### 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

Flammable liquids, Category 3  
Acute toxicity - Category 3, Oral  
Skin irritation, Category 2  
Eye irritation, Category 2  
Acute toxicity - Category 3, Inhalation  
Specific target organ toxicity – single exposure, Category 3

#### Label elements

##### Pictogram(s)

☐☐☐

Signal word : Danger

##### Hazard statement(s)

H226 Flammable liquid and vapour  
H315 Causes skin irritation  
H319 Causes serious eye irritation  
H335 May cause respiratory irritation

### **Precautionary statement(s)**

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

P233 Keep container tightly closed.

P240 Ground/bond container and receiving equipment.

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

P264 Wash hands thoroughly after handling.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P271 Use only outdoors or in a well-ventilated area.

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

P370+P378 In case of fire: Use ... for extinction.

P405 Store locked up.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P501 Dispose of contents/container to.....

### **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.

P270 Do not eat, drink or smoke when using this product.

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

P271 Use only outdoors or in a well-ventilated area.

### **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.

P301+P316 IF SWALLOWED: Get emergency medical help immediately.

P321 Specific treatment (see ... on this label).

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P332+P317 If skin irritation occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

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

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P316 Get emergency medical help immediately.

P319 Get medical help if you feel unwell.

### **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**

no data available

---

## SECTION 3: Composition/information on ingredients

#### **Substance**

Product name	: ISOTHIOCYANIC ACID 4-PENTEN-1-YL ESTER
Synonyms	: 4-PENTEN-1-YL ISOTHIOCYANATE,5-Isothiocyanato-1-pentene
CAS	: 18060-79-2
MF	: C6H9NS
MW	: 127.21

---

## SECTION 4: First aid measures

#### **Description of first aid measures**

##### **If inhaled**

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

##### **Following skin contact**

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

##### **Following eye contact**

Rinse with pure water for at least 15 minutes. Consult a doctor.

##### **Following ingestion**

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

#### **Most important symptoms and effects, both acute and delayed**

no data available

#### **Indication of any immediate medical attention and special treatment needed**

no data available

---

## SECTION 5: Firefighting measures

#### **Extinguishing media**

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

## Specific Hazards Arising from the Chemical

no data available

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

---

## 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

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

### Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

---

## 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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

---

## SECTION 8: Exposure controls/personal protection

### Control parameters

#### Occupational Exposure limit values

no data available

#### 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	Oil
Colour	Colourless
Odour	no data available
Melting point/freezing point	257°C(lit.)
Boiling point or initial boiling point and boiling range	194°C(lit.)
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	97°C(lit.)
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Chloroform (Soluble), Hexanes (Slightly)
Partition coefficient n-octanol/water	no data available
Vapour pressure	1.09mmHg at 25°C
Density and/or relative density	0.9g/cm <sup>3</sup>
Relative vapour density	no data available
Particle characteristics	no data available

---

## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

no data available

#### **Possibility of hazardous reactions**

no data available

#### **Conditions to avoid**

no data available

#### **Incompatible materials**

no data available

#### **Hazardous decomposition products**

no data available

---

## SECTION 11: Toxicological information

#### **Acute toxicity**

- Oral: no data available
- Inhalation: no data available
- 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**

no data available

#### **Reproductive toxicity**

no data available

#### **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: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

### **Persistence and degradability**

no data available

### **Bioaccumulative potential**

no data available

### **Mobility in soil**

no data available

### **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: UN1992 (For reference only, please check.)

IMDG: UN1992 (For reference only, please check.)

IATA: UN1992 (For reference only, please check.)

### **UN Proper Shipping Name**

ADR/RID: FLAMMABLE LIQUID, TOXIC, N.O.S. (For reference only, please check.)

IMDG: FLAMMABLE LIQUID, TOXIC, N.O.S. (For reference only, please check.)

IATA: FLAMMABLE LIQUID, TOXIC, N.O.S. (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: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

### **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)**

Not Listed.

#### **EC Inventory**

Not 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)**

Not Listed.

#### **PICCS**

Not Listed.

#### **Vietnam National Chemical Inventory**

Not 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?pageID=0&request\\_locale=en](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/>

#### **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.