

## Chemical Safety Data Sheet MSDS / SDS

**PENTAFLUOROPHENYL ISOCYANATE 97**

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

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

Product name : PENTAFLUOROPHENYL ISOCYANATE 97  
CBnumber : CB7500084  
CAS : 1591-95-3  
EINECS Number : 216-470-7  
Synonyms : PENTAFLUOROPHENYL ISOCYANATE 97

**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**

P342+P311 IF experiencing respiratory symptoms: 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.

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

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled

H332 Harmful if inhaled

H319 Causes serious eye irritation

H315 Causes skin irritation  
H312 Harmful in contact with skin  
H302 Harmful if swallowed

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## SECTION 3: Composition/information on ingredients

### Substance

Product name : PENTAFLUOROPHENYL ISOCYANATE 97  
Synonyms : PENTAFLUOROPHENYL ISOCYANATE 97  
CAS : 1591-95-3  
EC number : 216-470-7  
MF : C7F5NO  
MW : 209.07

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor

#### If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

### **Special hazards arising from the substance or mixture**

Carbon oxides Nitrogen oxides (NOx) Hydrogen fluoride Combustible.

Vapors are heavier than air and may spread along floors. Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

### **Advice for firefighters**

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### **Further information**

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## **SECTION 6: Accidental release measures**

### **Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

### **Environmental precautions**

Do not let product enter drains.

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

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g.

Chemisorb?). Dispose of properly. Clean up affected area.

### **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**

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

### **Hygiene measures**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

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

## Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

## Storage stability

Recommended storage temperature

2 - 8 °C

Store under inert gas. Moisture sensitive.

## 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

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

#### Skin protection

required

#### Body Protection

protective clothing

#### Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

#### Control of environmental exposure

Do not let product enter drains.

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# SECTION 9: Physical and chemical properties

## Information on basic physicochemical properties

Appearance	colorless liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	36 °C
Initial boiling point and boiling range	52 °C at 3 hPa - lit.
Flash point	110 °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	1,6 g/cm <sup>3</sup> at 25 °C - lit. 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

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### Possibility of hazardous reactions

No data available

### Conditions to avoid

Avoid moisture. Strong heating.

### Incompatible materials

Strong oxidizing agents

### 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

Acute toxicity estimate Oral - 500,1 mg/kg (Expert judgment)

Acute toxicity estimate Oral - Expert judgment - 500,1 mg/kg Acute toxicity estimate Inhalation - 4 h - 1,6 mg/l  
(Expert judgment)

Acute toxicity estimate Inhalation - Expert judgment - 4 h - 1,6 mg/l Acute toxicity estimate Dermal - 1.100,1 mg/kg  
(Expert judgment)

Acute toxicity estimate Dermal - Expert judgment - 1.100,1 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

No data available

#### 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**

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

### **UN number**

ADR/RID: 2206 IMDG: 2206 IATA: 2206

### **UN proper shipping name**

ADR/RID: ISOCYANATES, TOXIC, N.O.S. (Perfluorophenyl isocyanate) IMDG: ISOCYANATES, TOXIC, N.O.S. (Perfluorophenyl isocyanate)  
IATA: Isocyanates, toxic, n.o.s. (Perfluorophenyl isocyanate)

### **Transport hazard class(es)**

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

### **Packaging group**

ADR/RID: III IMDG: III IATA: III

### **Environmental hazards**

ADR/RID: no IMDG Marine pollutant: no 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**

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.

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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.