

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Phenyl isothiocyanate PEPTIPURE® ≥99 %, for biochemistry

article number: **7296**  
Version: **GHS 4.0 en**  
Replaces version of: 2023-07-03  
Version: (GHS 3)

date of compilation: 2021-02-18  
Revision: 2024-03-04

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

### 1.1 Product identifier

Identification of the substance	<b>Phenyl isothiocyanate</b> PEPTIPURE® ≥99 %, for biochemistry
Article number	7296
CAS number	103-72-0

### 1.2 Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses:	Isolated intermediate
Uses advised against:	Do not use for squirting or spraying. Do not use for products which come into direct contact with the skin. Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household). Food, drink and animal feedingstuffs.

### 1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG  
Schoemperlenstr. 3-5  
D-76185 Karlsruhe  
Germany

**Telephone:** +49 (0) 721 - 56 06 0  
**Telefax:** +49 (0) 721 - 56 06 149  
**e-mail:** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)  
**Website:** [www.carlroth.de](http://www.carlroth.de)

Competent person responsible for the safety data sheet: Department Health, Safety and Environment

**e-mail (competent person):** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

### 1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 Westmead, NSW	131126	

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

Classification acc. to GHS

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Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
2.6	Flammable liquid	4	Flam. Liq. 4	H227
3.10	Acute toxicity (oral)	3	Acute Tox. 3	H301
3.2	Skin corrosion/irritation	1B	Skin Corr. 1B	H314
3.4R	Respiratory sensitisation	1B	Resp. Sens. 1B	H334
3.4S	Skin sensitisation	1B	Skin Sens. 1B	H317

For full text of abbreviations: see SECTION 16

### The most important adverse physicochemical, human health and environmental effects

Skin corrosion produces an irreversible damage to the skin; namely, visible necrosis through the epidermis and into the dermis. The product is combustible and can be ignited by potential ignition sources.

## 2.2 Label elements

### Labelling

#### Signal word

**Danger**

#### Pictograms

GHS05, GHS06,  
GHS08



#### Hazard statements

H227	Combustible liquid
H301	Toxic if swallowed
H314	Causes severe skin burns and eye damage
H317	May cause an allergic skin reaction
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled

#### Precautionary statements

##### Precautionary statements - prevention

P260	Do not breathe dusts or mists
P280	Wear protective gloves/protective clothing/eye protection/face protection

##### Precautionary statements - response

P301+P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
P302+P352	IF ON SKIN: Wash with plenty of soap and water
P303+P361+P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P370+P378	In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction

## 2.3 Other hazards

This material is combustible, but will not ignite readily.

### Results of PBT and vPvB assessment

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According to the results of its assessment, this substance is not a PBT or a vPvB.

### Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	Phenyl isothiocyanate
Molecular formula	C <sub>7</sub> H <sub>5</sub> NS
Molar mass	135.2 g/mol
CAS No	103-72-0

## SECTION 4: First aid measures

### 4.1 Description of first aid measures



#### General notes

Take off immediately all contaminated clothing. Self-protection of the first aider.

#### Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

#### Following skin contact

After contact with skin, wash immediately with plenty of water. Immediate medical treatment required because corrosive injuries that are not treated are hard to cure. In case of skin reactions, consult a physician.

#### Following eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye.

#### Following ingestion

Rinse mouth immediately and drink plenty of water. Call a physician immediately. If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects).

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

Corrosion, Breathing difficulties, Cough, Risk of blindness, Gastric perforation, Vomiting, Allergic reactions, Nausea

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

none

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### SECTION 5: Firefighting measures

#### 5.1 Extinguishing media



##### Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!  
water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO<sub>2</sub>)

##### Unsuitable extinguishing media

water jet

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

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours may form explosive mixtures with air.

##### Hazardous combustion products

In case of fire may be liberated: Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Sulphur oxides (SO<sub>x</sub>), Hydrogen cyanide (HCN, prussic acid)

#### 5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus. Wear full chemical protective clothing.

### SECTION 6: Accidental release measures

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



##### For non-emergency personnel

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. Do not breathe vapour/spray. Avoidance of ignition sources.

#### 6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it. If substance has entered a water course or sewer, inform the responsible authority.

#### 6.3 Methods and material for containment and cleaning up

##### Advice on how to contain a spill

Covering of drains.

##### Advice on how to clean up a spill

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

##### Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

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### 6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Provision of sufficient ventilation. Handle and open container with care. Clear contaminated areas thoroughly.

#### Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge.

#### Advice on general occupational hygiene

When using do not eat or drink. Thorough skin-cleansing after handling the product.

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

Keep container tightly closed.

#### Incompatible substances or mixtures

Observe hints for combined storage.

#### Consideration of other advice:

Store locked up.

#### Ventilation requirements

Use local and general ventilation.

#### Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C

### 7.3 Specific end use(s)

No information available.

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### National limit values

#### Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

### 8.2 Exposure controls

#### Individual protection measures (personal protective equipment)

##### Eye/face protection



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Use safety goggles with side protection. Wear face protection.

### Skin protection



#### • hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. Check leak-tightness/impermeability prior to use. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 °C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

#### • type of material

NBR (Nitrile rubber)

#### • material thickness

>0,11 mm

#### • breakthrough times of the glove material

>480 minutes (permeation: level 6)

#### • other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

### Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C, colour code: Brown).

### Environmental exposure controls

Keep away from drains, surface and ground water.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	yellow
Odour	characteristic
Melting point/freezing point	-21 °C
Boiling point or initial boiling point and boiling range	221 °C at 1,013 hPa
Flammability	flammable liquid in accordance with GHS criteria
Lower and upper explosion limit	not determined

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Flash point	87 °C
Auto-ignition temperature	not determined
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	1.15 mm <sup>2</sup> /s at 20 °C
Dynamic viscosity	1.3 mPa s at 20 °C

### Solubility(ies)

Water solubility not determined

### Partition coefficient

Partition coefficient n-octanol/water (log value): 3.28 (Lit.)

Vapour pressure 10 hPa at 20 °C

### Density and/or relative density

Density 1.13 g/cm<sup>3</sup>

Relative vapour density 4.65 (air = 1)

Particle characteristics not relevant (liquid)

### Other safety parameters

Oxidising properties none

## 9.2 Other information

Information with regard to physical hazard classes: There is no additional information.

Other safety characteristics: There is no additional information.

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

It's a reactive substance. Risk of ignition.

#### **If heated**

Risk of ignition. Vapours may form explosive mixtures with air.

### 10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

### 10.3 Possibility of hazardous reactions

Material reacts vigorously with water emitting flammable gases,

**Violent reaction with:** Alcohols, Amines, Chlorates, Nitrate, Oxidisers, Acids, Water, Alkalines

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### 10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.  
Keep away from heat.

### 10.5 Incompatible materials

There is no additional information.

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Classification acc. to GHS

#### Acute toxicity

Toxic if swallowed.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	87 mg/kg	mouse		TOXNET

#### Skin corrosion/irritation

Causes severe skin burns and eye damage.

#### Serious eye damage/eye irritation

Causes serious eye damage.

#### Respiratory or skin sensitisation

May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause an allergic skin reaction.

#### Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

#### Carcinogenicity

Shall not be classified as carcinogenic.

#### Reproductive toxicity

Shall not be classified as a reproductive toxicant.

#### Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

#### Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

#### Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

#### Symptoms related to the physical, chemical and toxicological characteristics

##### • If swallowed

If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects)



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- **If in eyes**

causes burns, Causes serious eye damage, risk of blindness

- **If inhaled**

May produce an allergic reaction, cough, Dyspnoea

- **If on skin**

causes severe burns, causes poorly healing wounds, May produce an allergic reaction, pruritis, localised redness

- **Other information**

This information is based upon the present state of our knowledge.

### 11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.

## SECTION 12: Ecological information

### 12.1 Toxicity

Very toxic to aquatic life with long lasting effects.

### 12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 2.13 mg/mg

Theoretical Oxygen Demand (with nitrification): 2.604 mg/mg

Theoretical Carbon Dioxide: 2.279 mg/mg

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	3.28 (Lit.)
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### 12.4 Mobility in soil

Data are not available.

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.

### 12.7 Other adverse effects

Data are not available.

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

#### Sewage disposal-relevant information

Do not empty into drains.

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### Waste treatment of containers/packagings

Only packagings which are approved (e.g. acc. to the Dangerous Goods Regulations) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

### Relevant provisions relating to waste(Basel Convention)

#### Properties of waste which render it hazardous

H8 Corrosives

### 13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

## SECTION 14: Transport information

### 14.1 UN number

UN RTDG	UN 2922
IMDG-Code	UN 2922
ICAO-TI	UN 2922

### 14.2 UN proper shipping name

UN RTDG	CORROSIVE LIQUID, TOXIC, N.O.S.
IMDG-Code	CORROSIVE LIQUID, TOXIC, N.O.S.
ICAO-TI	Corrosive liquid, toxic, n.o.s.
Technical name	Phenyl isothiocyanate

### 14.3 Transport hazard class(es)

UN RTDG	8 (6.1)
IMDG-Code	8 (6.1)
ICAO-TI	8 (6.1)

### 14.4 Packing group

UN RTDG	II
IMDG-Code	II
ICAO-TI	II

### 14.5 Environmental hazards

hazardous to the aquatic environment

### 14.6 Special precautions for user

There is no additional information.

### 14.7 Transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

### 14.8 Information for each of the UN Model Regulations

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### Transport information National regulations Additional information (UN RTDG)

<b>UN number</b>	2922
<b>Class</b>	8
<b>Subsidiary risk(s)</b>	6.1
<b>Environmental hazards</b>	Yes Hazardous to the aquatic environment
<b>Packing group</b>	II
<b>Danger label(s)</b>	8+6.1 Fish and tree



<b>Special provisions (SP)</b>	274 UN RTDG
<b>Excepted quantities (EQ)</b>	E2 UN RTDG
<b>Limited quantities (LQ)</b>	1 L UN RTDG
<b>Emergency Action Code</b>	2X

### International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name	CORROSIVE LIQUID, TOXIC, N.O.S.
Particulars in the shipper's declaration	UN2922, CORROSIVE LIQUID, TOXIC, N.O.S., (Phenyl isothiocyanate), 8 (6.1), II, MARINE POLLUTANT
Marine pollutant	yes (hazardous to the aquatic environment)
Danger label(s)	8+6.1, "Fish and tree"



Special provisions (SP)	274
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
EmS	F-A, S-B
Stowage category	B

### International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Proper shipping name	Corrosive liquid, toxic, n.o.s.
Particulars in the shipper's declaration	UN2922, Corrosive liquid, toxic, n.o.s., (Phenyl isothiocyanate), 8 (6.1), II
Environmental hazards	yes (hazardous to the aquatic environment)
Danger label(s)	8+6.1



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Special provisions (SP)	A3, A4
Excepted quantities (EQ)	E2
Limited quantities (LQ)	0,5 L

### SECTION 15: Regulatory information

#### 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

There is no additional information.

##### National regulations(Australia)

##### Australian Inventory of Chemical Substances(AICS)

Substance is listed.

##### Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

##### National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
JP	ISHA-ENCS	substance is listed
KR	KECI	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

##### Legend

AIIC	Australian Inventory of Industrial Chemicals
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
ISHA-ENCS	Inventory of Existing and New Chemical Substances (ISHA-ENCS)
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

#### 15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

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### SECTION 16: Other information

#### Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.3	Endocrine disrupting properties: Does not contain an endocrine disruptor (EDC) in a concentration of ≥ 0,1%.	Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
15.1		National inventories: change in the listing (table)	yes

#### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative

#### Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

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### List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H227	Combustible liquid.
H301	Toxic if swallowed.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.

### Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.