

# SAFETY DATA SHEET

Version 6.1  
Revision Date 13.03.2021  
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## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : Phenyl isothiocyanate

Product Number : 78780  
Brand : Sigma-Aldrich  
CAS-No. : 103-72-0

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

Identified uses : Laboratory chemicals, Synthesis of substances

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

Company : SIGMA-ALDRICH CANADA LTD.  
2149 WINSTON PARK DRIVE  
OAKVILLE ON L6H 6J8  
CANADA

Telephone : +1 905 829-9500  
Fax : +1 905 829-9292

### 1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA)  
+1-703-527-3887 CHEMTREC  
(International)  
24 Hours/day; 7 Days/week

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### GHS Classification in accordance with Hazardous Products Regulations (HPR) (SOR/2015-17)

Flammable liquids (Category 4), H227  
Acute toxicity, Oral (Category 3), H301  
Skin corrosion (Category 1B), H314  
Serious eye damage (Category 1), H318  
Respiratory sensitization (Category 1), H334  
Skin sensitization (Category 1), H317  
Short-term (acute) aquatic hazard (Category 2), H401  
Long-term (chronic) aquatic hazard (Category 2), H411

For the full text of the H-Statements mentioned in this Section, see Section 16.

### 2.2 GHS Label elements, including precautionary statements

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Pictogram



Signal word

Danger

Hazard statement(s)

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.  
H411 Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.  
P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.  
P264 Wash skin thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P272 Contaminated work clothing should not be allowed out of the workplace.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.  
P284 Wear respiratory protection.  
P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.  
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.  
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.  
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.  
P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.  
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.  
P342 + P311 If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.  
P362 + P364 Take off contaminated clothing and wash it before reuse.  
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.  
P391 Collect spillage.  
P403 Store in a well-ventilated place.  
P405 Store locked up.  
P501 Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Lachrymator.

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

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Synonyms : PITC  
 Molecular weight : 135.19 g/mol  
 CAS-No. : 103-72-0  
 EC-No. : 203-138-1

Component	Classification	Concentration *
<b>Phenylisothiocyanate</b>		
	Flam. Liq. 4; Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Resp. Sens. 1; Skin Sens. 1; Aquatic Acute 2; Aquatic Chronic 2; H227, H301, H314, H318, H334, H317, H401, H411	<= 100 %
* Weight %		

For the full text of the H-Statements mentioned in this Section, see Section 16.

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Take off contaminated clothing and shoes immediately. 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. Continue rinsing eyes during transport to hospital.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 4.2 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

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

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

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

#### Unsuitable extinguishing media

Do NOT use water jet.

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

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Sulfur oxides

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

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## SECTION 6: Accidental release measures

### 6.1 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.

### 6.2 Environmental precautions

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

### 6.3 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.

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 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.

## 7.2 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.

### Storage stability

Recommended storage temperature

2 - 8 °C

Moisture sensitive.

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

## 7.3 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

### 8.1 Control parameters

### 8.2 Exposure controls

#### Appropriate engineering controls

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

#### Personal protective equipment

##### Eye/face protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). 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.

Full contact

Material: Fluorinated rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 30 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our

customers. It should not be construed as offering an approval for any specific use scenario.

### **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. Discharge into the environment must be avoided.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

- |   |  |
|---|--|
| a) Appearance                                   | Form: liquid<br>Color: colorless           |
| b) Odor   | No data available                          |
| c) Odor Threshold                               | No data available                          |
| d) pH   | No data available                          |
| e) Melting point/freezing point                 | Melting point/range: -21 °C (-6 °F) - lit. |
| f) Initial boiling point and boiling range      | 218 °C 424 °F - lit.                       |
| g) Flash point                                  | 88 °C (190 °F) - closed cup                |
| h) Evaporation rate                             | No data available                          |
| i) Flammability (solid, gas)                    | No data available                          |
| j) Upper/lower flammability or explosive limits | No data available                          |
| k) Vapor pressure                               | No data available                          |
| l) Vapor density                                | No data available                          |
| m) Relative density                             | No data available                          |
| n) Water solubility                             | insoluble                                  |
| o) Partition coefficient: n-octanol/water       | log Pow: > 3                               |
| p) Autoignition temperature                     | No data available                          |
| q) Decomposition                                | No data available                          |

temperature

- r) Viscosity No data available
- s) Explosive properties No data available
- t) Oxidizing properties No data available

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Water, Alcohols, Strong bases, Amines, acids, Strong oxidizing agents

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Mouse - 87 mg/kg

Remarks:

Kidney, Ureter, Bladder:Urine volume increased.

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

Mammal

Remarks:

Cytogenetic analysis

#### Carcinogenicity

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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.

ACGIH: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

**Reproductive toxicity**

No data available  
No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

RTECS: NX9275000

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache, Nausea

Stomach - Irregularities - Based on Human Evidence

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**SECTION 12: Ecological information**

**12.1 Toxicity**

Toxicity to daphnia and other aquatic invertebrates LC50 - Daphnia magna (Water flea) - 0.1 mg/l - 48 h

**12.2 Persistence and degradability**

No data available

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Other adverse effects**

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.  
Toxic to aquatic life.



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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Offer surplus and non-recyclable solutions to a licensed disposal company. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Contact a licensed professional waste disposal service to dispose of this material.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### TDG

UN number: 2927 Class: 6.1 (8) Packing group: II  
Proper shipping name: TOXIC LIQUID, CORROSIVE, ORGANIC, N.O.S.  
(Phenylisothiocyanate)  
Subsidiary risk : 8  
Labels: 6.1  
(8)ERG Code: 154  
Marine pollutant: no

### IMDG

UN number: 2927 Class: 6.1 (8) Packing group: II EMS-No: F-A, S-B  
Proper shipping name: TOXIC LIQUID, CORROSIVE, ORGANIC, N.O.S.  
(Phenylisothiocyanate)

### IATA

UN number: 2927 Class: 6.1 (8) Packing group: II  
Proper shipping name: Toxic liquid, corrosive, organic, n.o.s. (Phenylisothiocyanate)

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## SECTION 15: Regulatory information

This product has been classified in accordance with the hazard criteria of the Hazardous Products Regulations (HPR) and the SDS contains all the information required by the HPR.

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## SECTION 16: Other information

### Further information

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