

## Phenyl-d<sub>5</sub> Isothiocyanate

### Section 1. Chemical product and company identifications

**Product code:** D-5529

**Chemical formula:** C<sub>7</sub>D<sub>5</sub>NS

**CAS:** 74881-77-9

**CAS (unlabelled):** 103-72-0

**Synonyms:** Isothiocyanatobenzene, Phenyl Mustard Oil

**Supplier / Manufacturer:**

**C/D/N Isotopes Inc.**

88 Leacock Street

Pointe-Claire (Québec) H9R 1H1

Phone: 514-697-6254

Toll-Free (Canada & USA): 1-800-565-4696

Fax: 514-697-6148

Website: www.cdnisotopes.com

**In case of emergency:**

**TOXYSKAN HOTLINE: 1-855-780-0599**

### Section 2. Hazards identifications





**Physical state:** Liquid

**Warning:** Combustible liquid. Toxic if swallowed. Causes severe skin burns and eye damage.

**Routes of entry:** Inhalation, ingestion, skin and eyes

#### GHS (Globally Harmonized System of Classification and Labelling of Chemicals):

- GHS Classification:**
- Flammable liquids (Category 4)
  - Acute toxicity, Oral (Category 3)
  - Skin corrosion (Category 1B)
  - Serious eye damage (Category 1)
  - Respiratory sensitisation (Category 1)
  - Skin sensitisation (Category 1)

- GHS Label elements:**
- Pictograms:    
  - Signal word: Danger

- Hazards statement:**
- 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 statement:**
- P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
  - P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
  - P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
  - P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
  - P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
  - P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
  - P316 Get emergency medical help immediately.

### Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
Phenyl-d <sub>5</sub> Isothiocyanate	74881-77-9	> 98

## **Section 4. First aid measures**

**Eye contact:** Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**Skin contact:** Wash off with soap and plenty of water. Consult a physician.

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

**Ingestion:** Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

**General advice:** Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

## **Section 5. Firefighting measures**

**Flammability of the product:** Flammable in the presence of a source of ignition when the temperature is above the flash point. Keep away from heat/sparks/open flame/hot surface. No smoking.

**Lower explosion limit:** No data available.

**Upper explosion limit:** No data available.

**Auto-ignition temperature:** No data available.

**Flash point:** 88 °C (190 °F)

**Products of combustion:** Hazardous decomposition products formed under fire conditions: Carbon oxides, nitrogen oxides, sulfur oxides.

**Firefighting media and instructions:** Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

**Special protective equipment for firefighters:** Wear self-contained breathing apparatus for firefighting if necessary.

## **Section 6. Accidental release measures**

**Personal precautions:** Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition.

**Environmental precautions:** Do not let product enter drains. Discharge into the environment must be avoided.

**Methods for cleaning up:** Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

## **Section 7. Handling and storage**

**Handling:** Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Provide appropriate exhaust ventilation. Keep away from sources of ignition - No smoking.

**Storage:** Store at room temperature. Adequate ventilation. Protect from heat. Protect from moisture.

## **Section 8. Exposure Controls, Personal Protections**

**Engineering controls:** Use mechanical exhaust or laboratory fumehood to avoid exposure.

**Eyes:** Safety glasses with side-shields conforming to NIOSH (US) or EN 166 (EU).

**Respiratory:** 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).

**Hands:** Handle with gloves. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

**Skin/body:** Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

## **Section 9. Physical and chemical properties (unlabelled)**

**Molecular weight:** 135.19 g/mol

**Physical status:** Liquid

**Color:** Colorless to yellow

**Odour:** No data available

**Density:** 1.132 g/cm<sup>3</sup>

**Melting point:** -21 °C (-6 °F)

**Boiling point:** 218 °C (424 °F)

**Vapour pressure:** 2 hPa (1.5 mmHg) at 25 °C (77 °F)

**Vapour density:** 4.68 (Air = 1)

**Partition coefficient (octanol/water):** log Pow: 3.28

**Water solubility:** 90 mg/L

## **Section 10. Stability and reactivity**

**Stability and reactivity:** Stable under recommended storage conditions.

**Incompatibility:** Water, alcohols, strong bases, amines, acids, strong oxidizing agents.

**Products of combustion:** Hazardous decomposition products formed under fire conditions: Carbon oxides, nitrogen oxides, sulfur oxides.

**Reactivity conditions:** Heat, flames and sparks. Avoid moisture.

## **Section 11. Toxicological information (unlabelled)**

**Toxicological data:** Phenyl Isothiocyanate

### **Information on ingredients:**

<b><u>Name</u></b>	<b><u>CAS</u></b>	<b><u>LD<sub>50</sub></u></b>	<b><u>LC<sub>50</sub></u></b>
Phenyl Isothiocyanate	103-72-0	Oral - Mouse - 87 mg/kg	No data available

### **Potential acute effects**

- **Eyes:** Causes severe eye damage.
- **Skin:** May be harmful if absorbed through skin. Causes severe skin burns. May cause an allergic skin reaction.
- **Inhalation:** May be harmful if inhaled. May cause respiratory tract irritation. May cause allergy or asthma symptoms or breathing difficulties if inhaled.
- **Ingestion:** Toxic if swallowed.

### **Potential chronic effects**

- **Carcinogenic effects:** IARC: No component 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 component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- **Mutagenic effects:** Genotoxicity in vivo - Mammal - Skin. Cytogenetic analysis.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

## **Section 12. Ecological information**

### **Ecological data:**

<b><u>Name</u></b>	<b><u>Results</u></b>	<b><u>Species</u></b>	<b><u>Period</u></b>
Phenyl Isothiocyanate	0.1 mg/l LC50	Daphnia magna	48 h

**Effects on environment:** An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

**Mobility:** No data available.

**Environmental precautions:** No data available.

**Persistence and degradability:** No data available.

**Bioaccumulative potential:** No data available.

## **Section 13. Disposal considerations**

**Waste disposal:** Contact a licensed professional waste disposal service to dispose of this material.

## **Section 14. Transportation information**

### **Classification DOT/IMDG/IATA label:**

**Shipping name:** Toxic liquids, corrosive, organic, n.o.s. (Phenyl isothiocyanate)

**UN number:** UN2927

**Class:** 6.1 (8)

**Packaging group:** II

**Additional information:** None

## **Section 15. Regulatory information**

### **UNITED STATES: NFPA classification**



Health: 3  
Flammable: 2  
Reactivity: 0  
Special conditions: None

**Legend: 4: Severe, 3: High, 2: Moderate, 1: Slightly, 0: Not hazardous**

### **U.S. Federal regulations:**

**TSCA 8(b) inventory:** Phenyl Isothiocyanate

**SARA 302/304/311/312 extremely hazardous substances:** Not Listed

**SARA 302/304 emergency planning and notification:** Not Listed

**SARA 302/304/311/312 hazardous chemicals:** Not Listed

**SARA 311/312 MSDS distribution - chemical inventory - hazard identification:** Fire hazard, Immediate (acute) health hazard, Delayed (chronic) health hazard: Not Listed

**CWA (Clean Water Act) 307:** Not Listed

**CWA (Clean Water Act) 311:** Not Listed

**CAA (Clean Air Act) 112 accidental release prevention:** Not Listed

**CAA (Clean Air Act) 112 regulated flammable substances:** Not Listed

**CAA (Clean Air Act) 112 regulated toxic substances:** Not Listed

### **State regulations:**

**DEA List I Chemicals (Precursor Chemicals):** Not Listed

**DEA List II Chemicals (Essential Chemicals):** Not Listed

**Substances in Massachusetts:** Not Listed

**Dangerous substances in New Jersey:** Not Listed

**New York – Dangerous substances with acute effects:** Not Listed

**Dangerous substances in Pennsylvania – right to know:** Not Listed

### **WHMIS (Canada):**



B3 - Combustible liquid



D1B - Toxic material causing immediate and serious toxic effects



E - Corrosive material

## **Section 16. Additional information**

### **References:**

- ANSI Z400.1, MSDS Standard, 2001.
- Manufacturer's Material Safety Data Sheet.
- 29CFR Part1910.1200 OSHA MSDS Requirements.
- 49CFR Table List of Hazardous Materials, UN#, Proper Shipping Names, PG. -Canada
- Gazette Part II, Vol. 122, No. 2 Registration SOR/88-64 31 December, 1987 Hazardous Products Act "Ingredient Disclosure List".
- Federal act on the controlled products
- Canadian Transport of Dangerous Goods, Regulations and Schedules, Clear Language version 2002.
- Toxicological repertory, HSC.
- Material safety data sheet from the components.

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**Elaborated by: Toxyscan Inc., 1-866-780-0599**

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