

2-Phenyl-d₅-ethyl Isothiocyanate

Section 1. Chemical product and company identifications

Product code: D-7251

Chemical formula: C₉H₄D₅NS

CAS: 912627-98-6

CAS (unlabelled): 2257-09-2

Synonyms: Phenethyl Isothiocyanate

Supplier / Manufacturer:

C/D/N Isotopes Inc.

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In case of emergency:

TOXYSKAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

Physical state: Liquid

Warning: Harmful if swallowed, in contact with skin or inhaled. Causes skin irritation. Causes serious eye irritation.

Routes of entry: Inhalation, ingestion, skin and eyes

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

GHS Classification:

- Acute toxicity, Oral (Category 4)
- Acute toxicity, Dermal (Category 4)
- Acute toxicity, Inhalation (Category 4)
- Skin irritation (Category 2)
- Eye irritation (Category 2A)
- Respiratory sensitisation (Category 1)
- Skin sensitisation (Category 1)
- Specific target organ toxicity - single exposure (Category 3), Respiratory system

GHS Label elements:

- Pictograms:  
- Signal word: Danger

Hazards statement:

- H302 + H312 + H332 Harmful if swallowed, in contact with skin or inhaled.
- H315 Causes skin irritation.
- H317 May cause an allergic skin reaction.
- H319 Causes serious eye irritation.
- H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.
- H335 May cause respiratory irritation.

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 + P350 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.
- P342 + P316 If experiencing respiratory symptoms: Get emergency medical help immediately.
- P317 Get medical help.

Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
2-Phenyl-d ₅ -ethyl Isothiocyanate	912627-98-6	> 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: Not flammable or combustible.

Lower explosion limit: No data available.

Upper explosion limit: No data available.

Auto-ignition temperature: No data available.

Flash point: No data available.

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.

Environmental precautions: Do not let product enter drains.

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.

Storage: Store at room temperature. Adequate ventilation. 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: 163.24 g/mol

Physical status: Liquid

Color: Colorless to yellow

Odour: No data available

Density: 1.094 g/cm³

Melting point: No data available

Boiling point: 139 - 140 °C (282 - 284 °F) at 15 hPa (11 mmHg)

Vapour pressure: No data available

Vapour density: No data available

Partition coefficient (octanol/water): No data available

Water solubility: No data available

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.

Incompatibility: Strong oxidizing agents, strong acids, strong bases.

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

Reactivity conditions: Heat. Avoid moisture.

Section 11. Toxicological information (unlabelled)

Toxicological data: 2-Phenylethyl Isothiocyanate

Information on ingredients:

<u>Name</u>	<u>CAS</u>	<u>LD₅₀</u>	<u>LC₅₀</u>
2-Phenylethyl Isothiocyanate	2257-09-2	Oral - Mouse - 700 mg/kg	No data available

Potential acute effects

- **Eyes:** Causes serious eye irritation.
- **Skin:** Harmful if absorbed through skin. Causes skin irritation. May cause an allergic skin reaction.
- **Inhalation:** Harmful if inhaled. May cause respiratory tract irritation. May cause allergy or asthma symptoms or breathing difficulties if inhaled.
- **Ingestion:** Harmful 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:** In vivo tests showed mutagenic effects.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

Section 12. Ecological information

Ecological data:

<u>Name</u>	<u>Results</u>	<u>Species</u>	<u>Period</u>
2-Phenylethyl Isothiocyanate	0.13 mg/l LC50	Daphnia magna	48 h

Effects on environment: No data available.

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: Isocyanates, toxic, n.o.s. (Phenethyl Isothiocyanate)

UN number: 2206

Class: 6.1

Packaging group: III

Additional information: None

Section 15. Regulatory information

UNITED STATES: NFPA classification



Health: 2
Flammable: 0
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: 2-Phenylethyl 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):



D2A - Very toxic material causing other toxic effects
D2B - Toxic material causing other toxic effects

Section 16. Additional information

References:

- ANSI Z400.1, MSDS Standard, 2001.
- Manufacturer's Material Safety Data Sheet.
- 29CFR Part 1910.1200 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.

Date of issue: June 22nd, 2021

Version: 3

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

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