



Ethyl 4-Isocyanatobenzoate-2,3,5,6-d4

Section 1. Chemical product and company identifications

Product code: D-5970 Chemical formula: C₁₀H₅D₄NO₃ CAS: 1219802-91-1 CAS (unlabelled): 30806-83-8 Synonyms: 4-Ethoxycarbonylphenyl Isocyanate

Supplier / Manufacturer:

C/D/N Isotopes Inc.

In case of emergency: TOXYSCAN HOTLINE: 1-855-780-0599

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

Section 2. Hazards identifications

Physical state: Liquid or low melting solid 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) Specific target organ toxicity - single exposure (Category 3), Respiratory system
GHS Label elements:	- Pictograms:
Hazards statement:	 H302 + H312 + H332 Harmful if swallowed, in contact with skin or inhaled. H315 Causes skin irritation. 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>	Concentration %
Ethyl 4-Isocyanatobenzoate-2,3,5,6-d ₄	1219802-91-1	> 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.

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. **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 dust formation. Ensure adequate ventilation. Avoid breathing dust.

Environmental precautions: Do not let product enter drains.

Methods for cleaning up: Pick up and arrange disposal without creating dust. Keep in suitable, closed containers for disposal.

Section 7. Handling and storage

Handling: Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation. **Storage:** STORE REFRIGERATED. 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: 191.18 g/mol Physical status: White solid/colorless liquid Odour: No data available Density: 1.154 g/cm³ Melting point: 27 - 29 °C (81 - 84 °F) Boiling point: 118 - 119 °C (244 - 246 °F) at 1.1 hPa (0.8 mmHg) Vapour pressure: No data available Vapour density: No data available Partition coefficient (octanol/water): No data available Water solubility: Decomposes

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions. **Incompatibility:** Strong oxidizing agents, water, alcohols, amines, strong bases, acids. **Products of combustion:** Hazardous decomposition products formed under fire conditions: Carbon oxides, nitrogen oxides. **Reactivity conditions:** Avoid moisture.

Section 11. Toxicological information (unlabelled)

Toxicological data: Ethyl 4-Isocyanatobenzoate

Information on ingredients:

Name	<u>CAS</u>	<u>LD₅₀</u>	<u>LC₅₀</u>
Ethyl 4-Isocyanatobenzoate	30806-83-8	No data available	No data available

Potential acute effects

- Eyes: Causes serious eye irritation.
- Skin: Harmful if absorbed through skin. Causes skin irritation.
- 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: No data available.
- Teratogenic effects: No data available.
- Medical conditions aggravated by overexposure: No data available.

Section 12. Ecological information

Ecological data:

<u>Name</u>	Results	<u>Species</u>	Period		
Ethyl 4-Isocyanatobenzoate	No data available				
Effects on environment: No data available.					

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. (Ethyl 4-Isocyanatobenzoate) UN number: UN2206 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: Ethyl 4-Isocyanatobenzoate 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 CWA (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):

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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 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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