



## 3-Nitrobenzoic-d<sub>4</sub> Acid

### Section 1. Chemical product and company identifications

**Product code:** D-6440  
**Chemical formula:** C<sub>7</sub>HD<sub>4</sub>NO<sub>4</sub>  
**CAS:** 78399-78-7  
**CAS (unlabelled):** 121-92-6  
**Synonyms:** *m*-Nitrobenzoic Acid

**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:** Solid  
**Warning:** Harmful if swallowed. 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)
  - Skin irritation (Category 2)
  - Eye irritation (Category 2A)
  - Specific target organ toxicity - single exposure (Category 3), Respiratory system
- GHS Label elements:**
- Pictograms: 
  - Signal word: Warning
- Hazards statement:**
- H302 Harmful if swallowed.
  - H315 Causes skin irritation.
  - H319 Causes serious eye irritation.
  - 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 + P 330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
  - P302 + P350 IF ON SKIN: Wash with plenty of soap and water.
  - P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
  - P317 Get medical help.

### Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
3-Nitrobenzoic-d <sub>4</sub> Acid	78399-78-7	> 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:** Combustible at high temperature.

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

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

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

**Flash point:** 190 °C (374 °F)

**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. Discharge into the environment must be avoided.

**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 at room temperature. Adequate ventilation.

## **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:** 167.12 g/mol

**Physical status:** Solid

**Color:** Pale yellow

**Odour:** No data available

**Density:** No data available

**Melting point:** 139 - 141 °C (282 - 286 °F)

**Boiling point:** No data available

**Vapour pressure:** No data available

**Vapour density:** No data available

**Partition coefficient (octanol/water):** log Pow: 1.83

**Water solubility:** 3.6 g/L

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

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

**Incompatibility:** Strong oxidizing agents.

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

**Reactivity conditions:** No data available.

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

**Toxicological data:** 3-Nitrobenzoic Acid

### **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>
3-Nitrobenzoic Acid	121-92-6	Oral - Mouse - 1,450 mg/kg	No data available

### **Potential acute effects**

- **Eyes:** Causes serious eye irritation.
- **Skin:** May be harmful if absorbed through skin. Causes skin irritation.
- **Inhalation:** May be harmful if inhaled. May cause respiratory tract irritation.
- **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:** Genotoxicity in vitro - Ames test - S. typhimurium - with and without metabolic activation - negative.
- **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>
3-Nitrobenzoic Acid	50 mg/l LC50	Oryzias latipes	96 h
	71.3 mg/l EC50	Daphnia magna	48 h
	106.4 mg/l EC50	Desmodesmus subspicatus	72 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:** Aerobic. Result: 73.3 % - Readily biodegradable. Method: OECD Test guideline 301D.

**Bioaccumulative potential:** Cyprinus carpio - 6 weeks - 0.03 mg/l. Bioconcentration factor (BCF): 7.1.

## **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:** Not dangerous goods

**UN number:** None

**Class:** None

**Packaging group:** None

**Additional information:** None

## **Section 15. Regulatory information**

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



Health: 2  
Flammable: 1  
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:** 3-Nitrobenzoic Acid

**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):**



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.

**Date of issue:** February 9th, 2021

**Version:** 3

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

**Notice to reader:** To the best of our knowledge, the information contained herein is accurate. However, C/D/N Isotopes Inc., Toxyscan Inc., or any of its subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.