



## 4-Nitrotoluene-2,3,5,6-d<sub>4</sub>

### Section 1. Chemical product and company identifications

**Product code:** D-7322

**Chemical formula:** C<sub>7</sub>H<sub>3</sub>D<sub>4</sub>NO<sub>2</sub>

**CAS:** 1276197-16-0

**CAS (unlabelled):** 99-99-0

**Synonyms:** 1-Methyl-4-nitrobenzene

**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:** Toxic if swallowed, in contact with skin or if inhaled.

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

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

**GHS Classification:**

- Acute toxicity, Oral (Category 3)
- Acute toxicity, Inhalation (Category 3)
- Acute toxicity, Dermal (Category 3)
- Specific target organ toxicity - repeated exposure (Category 2)

**GHS Label elements:**

- Pictograms:  
- Signal word: Danger

**Hazards statement:**

- H301 + H311 + H331 Toxic if swallowed, in contact with skin or if inhaled
- H373 May cause damage to organs through prolonged or repeated exposure.

**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.
- P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
- P311 Call a POISON CENTER or doctor/ physician.

### Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
4-Nitrotoluene-2,3,5,6-d <sub>4</sub>	1276197-16-0	> 98

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

**Eye contact:** Flush eyes with water as a precaution.

**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:** 1.6 Vol%

**Upper explosion limit:** No data available

**Auto-ignition temperature:** 450 °C (842 °F)

**Flash point:** 106 °C (223 °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:** Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

**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.

**Methods for cleaning up:** Pick up and arrange disposal without creating dust. Sweep up and shovel. 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 at places where dust is formed.

**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).

**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:** 137.14 g/mol

**Physical status:** Solid

**Color:** Yellow

**Odour:** No data available

**Density:** 1.392 g/cm<sup>3</sup>

**Melting point:** 52 - 54 °C (126 - 129 °F)

**Boiling point:** 238 °C (460 °F)

**Vapour pressure:** 0.13 hPa (0.10 mmHg) at 20 °C (68 °F)

**Vapour density:** 5.49 (Air = 1)

**Partition coefficient (octanol/water):** log Pow: 2.37

**Water solubility:** 0.345 g/L

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

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

**Incompatibility:** Oxidizing agents, reducing agents, strong bases.

**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:** 4-Nitrotoluene

**Information on ingredients:**

<b>Name</b>	<b>CAS</b>	<b>LD<sub>50</sub></b>	<b>LC<sub>50</sub></b>
4-Nitrotoluene	99-99-0	Oral - Rat - 1,960 mg/kg Dermal - Rat - > 16,000 mg/kg	Inhalation - Rat - 975 mg/m <sup>3</sup>

### **Potential acute effects**

- **Eyes:** May cause eye irritation.
- **Skin:** Toxic if absorbed through skin. May cause skin irritation.
- **Inhalation:** Toxic if inhaled. May cause respiratory tract irritation.
- **Ingestion:** Toxic if swallowed.

### **Potential chronic effects**

- **Carcinogenic effects:** IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (4-Nitrotoluene). 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. Genotoxicity in vivo - Rat - male - Intraperitoneal - negative.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

## **Section 12. Ecological information**

**Ecological data:**

<b>Name</b>	<b>Results</b>	<b>Species</b>	<b>Period</b>
4-Nitrotoluene	49.7 mg/l LC50	<i>Pimephales promelas</i>	96 h
	4.2 mg/l EC50	<i>Daphnia magna</i>	48 h
	22 mg/l EC50	<i>Chlorella pyrenoidosa</i>	96 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:** According to the results of tests of biodegradability this product is not readily biodegradable.

**Bioaccumulative potential:** No data available.

## **Section 13. Disposal considerations**

**Waste disposal:** Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

## **Section 14. Transportation information**

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

**Shipping name:** Nitrotoluenes, solid

**UN number:** UN3446

**Class:** 6.1

**Packaging group:** II

**Additional information:** None

## **Section 15. Regulatory information**

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



Health: 2  
Flammable: 1  
Reactivity: 0  
Specials conditions:

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

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

**TSCA 8(b) inventory:** 4-Nitrotoluene

**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):**



D1A - Very toxic material causing immediate and serious toxic effects

D1B - Toxic material causing immediate and serious 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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