

4-Nitrotoluene-2,3,5,6-d₄

Section 1. Chemical product and company identifications

Product code: D-7322

Chemical formula: C₇H₃D₄NO₂

CAS: 1276197-16-0

CAS (unlabelled): 99-99-0

Synonyms: 1-Methyl-4-nitrobenzene

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: Solid

Warning: Harmful if swallowed. Fatal if inhaled.

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, Inhalation (Category 2)
 - Specific target organ toxicity - repeated exposure (Category 2)

GHS Label elements:

- Pictograms:   
- Signal word: Danger

Hazards statement:

- H302 Harmful if swallowed.
- H330 Fatal if inhaled.
- H373 May cause damage to organs through prolonged or repeated exposure.

Precautionary statement:

- P260 Do not breathe 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.
- P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
- P316 Get emergency medical help immediately.

Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
4-Nitrotoluene-2,3,5,6-d ₄	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: Flammable in the presence of a source of ignition when the temperature is above the flash point.

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 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).

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/cm³

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: 0.35 g/L

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.

Incompatibility: Strong oxidizing/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:

<u>Name</u>	<u>CAS</u>	<u>LD₅₀</u>	<u>LC₅₀</u>
4-Nitrotoluene	99-99-0	Oral - Rat - 1,960 mg/kg Dermal - Rat - > 16,000 mg/kg	Inhalation - Rat - 975 mg/m ³ Inhalation - Mouse - 419 mg/m ³

Potential acute effects

- **Eyes:** May cause eye irritation.
- **Skin:** May be harmful if absorbed through skin. May cause skin irritation.
- **Inhalation:** Fatal if inhaled. May cause respiratory tract irritation.
- **Ingestion:** Harmful 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:** May cause damage to organs through prolonged or repeated exposure.

Section 12. Ecological information

Ecological data:

<u>Name</u>	<u>Results</u>	<u>Species</u>	<u>Period</u>
4-Nitrotoluene	37 mg/l LC50	<i>Oryzias latipes</i>	96 h
	4.3 mg/l EC50	<i>Daphnia magna</i>	48 h
	5.5 mg/l EC50	<i>Selenastrum capricornutum</i>	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: 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: Contact a licensed professional waste disposal service to dispose of this material.

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: 3
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: 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: 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: Listed

Dangerous substances in New Jersey: Listed

New York – Dangerous substances with acute effects: Not Listed

Dangerous substances in Pennsylvania – right to know: Listed

WHMIS (Canada):



D1A - Very toxic material causing immediate and serious toxic effects



D2A - Very 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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