Safety Data Sheet

2-Nitrotoluene-d_7

Section 1. Chemical product and company identifications

Product code: D-7689
Chemical formula: $C_7D_7NO_2$
CAS: 84344-04-7
CAS (unlabelled): 88-72-2
Synonyms: *o*-Nitrotoluene, 1-Methyl-2-nitrobenzene

Supplier / Manufacturer:

C/D/N Isotopes Inc.
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In case of emergency:

TOXYSCAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

Physical state: Liquid
Warning: Harmful if swallowed.
Routes of entry: Inhalation, skin and eyes

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

GHS Classification:
- Acute toxicity, Oral (Category 4)
- Germ cell mutagenicity (Category 1B)
- Carcinogenicity (Category 1B)
- Reproductive toxicity (Category 2)

GHS Label elements:
- Pictograms:
- Signal word: Warning

Hazards statement:
- H302 Harmful if swallowed.
- H340 May cause genetic defects.
- H350 May cause cancer.
- H361 Suspected of damaging fertility or the unborn child.

Precautionary statement:
- P281 Use personal protective equipment as required.
- P308 + P313 IF exposed or concerned: Get medical advice/ attention.

Section 3. Composition and information on ingredients

Name	CAS	Concentration %
2-Nitrotoluene-d_7	84344-04-7	> 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.

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Section 5. Firefighting measures

Flammability of the product: Not flammable or combustible.
Lower explosion limit: 2.2 Vol%
Upper explosion limit: No data available.
Auto-ignition temperature: 420 °C (788 °F)
Flash point: 95 °C (203 °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 breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.
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: 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.
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: Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as 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: 137.14 g/mol
Physical status: Liquid
Color: Yellow
Odour: No data available
Density: 1.163 g/cm^3
Melting point: -4 °C (25 °F)
Boiling point: 222 °C (431 °F)
Vapour pressure: 0.16 hPa (0.12 mmHg) at 20 °C (68 °F)
Vapour density: 4.73 - (Air = 1)
Partition coefficient (octanol/water): log Pow: 2.3
Water solubility: 0.44 g/L at 20 °C (68 °F)

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.
Incompatibility: Oxidizing agents, strong bases.
Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides, nitrogen oxides.
Reactivity conditions: No data available.

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Section 11. Toxicological information (unlabelled)

Toxicological data: 2-Nitrotoluene

Information on ingredients:

Name	CAS	LD_{50}	LC_{50}
2-Nitrotoluene	88-72-2	Oral - Rat - 891 mg/kg	Inhalation - Rat - 790 mg/m^3

Potential acute effects

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

Potential chronic effects

- **Carcinogenic effects:** Carcinogenicity - Rat - male and female – Oral. Adenofibrosis. This product is or contains a component that has been reported to be probably carcinogenic based on its IARC, OSHA, ACGIH, NTP, or EPA classification. Possible human carcinogen. IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (2-Nitrotoluene). 3 - Group 3: Not classifiable as to its carcinogenicity to humans (2-Nitrotoluene). 2A - Group 2A: Probably carcinogenic to humans (2-Nitrotoluene). IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (2-Nitrotoluene). 3 - Group 3: Not classifiable as to its carcinogenicity to humans (2-Nitrotoluene). 2A - Group 2A: Probably carcinogenic to humans (2-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:** May alter genetic material. In vivo tests showed mutagenic effects. Genotoxicity in vitro - Hamster - fibroblast - with and without metabolic activation – positive. Genotoxicity in vivo - Rat - male - Oral – positive. DNA damage.
- **Teratogenic effects:** Suspected human reproductive toxicant.
- **Medical conditions aggravated by overexposure:** Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis.

Section 12. Ecological information

Ecological data:

Name	Results	Species	Period
2-Nitrotoluene	5.4 mg/l EC50	Daphnia magna	48 h
	22 mg/l EC50	Chlorella pyrenoidosa	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: No data available.
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, liquid
UN number: UN1664
Class: 6.1
Packaging group: II

Additional information: None

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Section 15. Regulatory information

UNITED STATES:
NFPA classification

Health: 1
Flammable: 1
Reactivity: 0
Specials conditions: None

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

U.S. Federal regulations:

TSCA 8(b) inventory: 2-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):

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.

Date of issue: **May 30th, 2017**
Version: 1
Elaborated by: **Toxyscan Inc., 1-866-780-0599**
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