



1-Bromooctane-3,3,4,4-d₄

Section 1. Chemical product and company identifications

Product code: D-7133

Chemical formula: C₈H₁₃D₄Br

CAS: 1219803-37-8

CAS (unlabelled): 111-83-1

Synonyms: *n*-Octyl Bromide

Supplier / Manufacturer:

C/D/N Isotopes Inc.

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Pointe-Claire (Québec) H9R 1H1
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Toll-Free (Canada & USA): 1-800-565-4696
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Website: www.cdnisotopes.com

In case of emergency:

TOXYSKAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

Physical state: Liquid

Warning: Combustible liquid. Causes skin irritation. Causes serious eye irritation.

Routes of entry: Inhalation, skin and eyes

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

GHS Classification:

- Flammable liquids (Category 4)
- Acute toxicity, Oral (Category 5)
- Skin corrosion/irritation (Category 2)
- Serious eye damage/eye irritation (Category 2A)
- Specific target organ toxicity - single exposure (Category 3), Respiratory system

GHS Label elements:

- Pictograms: 
- Signal word: Warning

Hazards statement:

- H227 Combustible liquid.
- H315 Causes skin irritation.
- H319 Causes serious eye irritation.
- H335 May cause respiratory irritation.

Precautionary statement:

- P210 Keep away from heat/sparks/open flame/hot surface. No smoking.
- P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
- P280 Wear protective gloves/ eye protection/ face protection.

Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
1-Bromooctane-3,3,4,4-d ₄	1219803-37-8	> 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: Do NOT induce vomiting. 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. Keep away from heat/sparks/open flame/hot surface. No smoking.

Lower explosion limit: No data available.

Upper explosion limit: No data available.

Auto-ignition temperature: No data available.

Flash point: 79 °C (174 °F)

Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides, hydrogen bromide gas.

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. Remove all sources of ignition. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low 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: Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

Section 7. Handling and storage

Handling: Avoid inhalation of vapour or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the build-up of electrostatic charge.

Storage: Store at room temperature. Adequate ventilation. Protect from heat and ignition sources.

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: 193.13 g/mol

Physical status: Liquid

Color: Colourless to pale yellow

Odour: No data available

Density: 1.118 g/mL at 25 °C (77 °F)

Melting point: -55 °C (-67 °F)

Boiling point: 201 °C (394 °F) - lit.

Vapour pressure: 0.45 hPa (0.34 mmHg) at 25 °C (77 °F)

Vapour density: 6.67 (Air = 1)

Partition coefficient (octanol/water): log Pow: 4.89

Water solubility: 1.67 mg/L

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.

Incompatibility: Strong oxidizing agents, Strong bases.

Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides, hydrogen bromide gas.

Reactivity conditions: Heat, flames and sparks.

Section 11. Toxicological information (unlabelled)

Toxicological data: 1-Bromooctane

Information on ingredients:

<u>Name</u>	<u>CAS</u>	<u>LD₅₀</u>	<u>LC₅₀</u>
1-Bromooctane	111-83-1	Oral - Rat - 4,984 mg/kg Dermal - Rabbit - 8,880 mg/kg	No data available

Potential acute effects

- **Eyes:** May cause eye irritation.
- **Skin:** May be harmful if absorbed through skin. May cause skin irritation.
- **Inhalation:** May be harmful if inhaled. May cause respiratory tract irritation.
- **Ingestion:** May be 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>	<u>Results</u>	<u>Species</u>	<u>Period</u>
1-Bromooctane	0.838 mg/l LC50	Pimephales promelas	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: No data available.

Bioaccumulative potential: No data available.

Section 13. Disposal considerations

Waste disposal: This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company.

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: 1
Flammable: 2
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: 1-Bromooctane

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):



B3 – Combustible liquid

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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