Safety Data Sheet

n-Hexadecyltrimethyl-d_3-ammonium Bromide (mono-methyl-d_3)

Section 1. Chemical product and company identifications

Product code: D-5744
Chemical formula: $C_{19}H_{39}D_3BrN$
CAS: 1092921-73-7
CAS (unlabelled): 57-09-0
Synonyms: Cetyltrimethylammonium Bromide, Palmityltrimethylammonium Bromide, Cetrimonium Bromide

Supplier / Manufacturer:

C/D/N Isotopes Inc.
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Toll-Free (Canada & USA): 1-800-565-4696
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Website: www.cdnisotopes.com

In case of emergency:

TOXYSCAN 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, 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.
- 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.

Section 3. Composition and information on ingredients

Name	CAS	Concentration %
n-Hexadecyltrimethyl-d_3-ammonium Bromide	1092921-73-7	> 98

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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: Not flammable or combustible.
Lower explosion limit: No data available.
Upper explosion limit: No data available.
Auto-ignition temperature: No data available.
Flash point: No data available.
Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides, nitrogen 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 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. Protect from moisture.

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: 364.45 g/mol
Physical status: Solid
Color: White to off-white
Odour: No data available
Density: No data available
Melting point: 248 - 251 °C (478 - 484 °F)
Boiling point: No data available
Vapour pressure: No data available
Vapour density: No data available
Partition coefficient (octanol/water): No data available
Water solubility: Soluble

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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, hydrogen bromide gas.
Reactivity conditions: No data available.

Section 11. Toxicological information (unlabelled)

Toxicological data: Hexadecyltrimethylammonium Bromide

Information on ingredients:

Name	CAS	LD_{50}	LC_{50}
Hexadecyltrimethylammonium Bromide	57-09-0	Oral - Rat - 410 mg/kg	No data available

Potential acute effects

- **Eyes:** Causes eye irritation.
- **Skin:** May be harmful if absorbed through skin. Causes skin irritation.
- **Inhalation:** May be harmful if inhaled.
- **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:** No data available.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

Section 12. Ecological information

Ecological data:

Name	Results	Species	Period
Hexadecyltrimethylammonium Bromide	0.3 mg/l LC50	Danio rerio	96 h
	0.03 mg/l EC50	Daphnia magna	48 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: Due to the distribution coefficient n-octanol/water, accumulation in organisms is not expected.

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: Not dangerous goods
UN number: None
Class: None
Packaging group: None

Additional information: None

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Section 15. Regulatory information

UNITED STATES:
NFPA classification

Health: 2
Flammable: 1
Reactivity: 1
Specials conditions: None

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

U.S. Federal regulations:

TSCA 8(b) inventory: Hexadecyltrimethylammonium Bromide
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: 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.

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