Safety Data Sheet

Hexachloro-1,3-butadiene-$^{13}C_4$

Section 1. Chemical product and company identifications

Product code: C-2408
Chemical formula: $^{13}C_4Cl_6$
CAS: 93951-70-3
CAS (unlabelled): 87-68-3
Synonyms: Hexachlorobutadiene, Perchlorobutadiene

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: Toxic if swallowed. Fatal in contact with skin or inhaled. Causes skin irritation. Causes serious eye damage.
Routes of entry: Inhalation, ingestion, skin and eyes

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

GHS Classification:
- Acute toxicity, Oral (Category 3)
- Acute toxicity, Dermal (Category 2)
- Acute toxicity, Inhalation (Category 2)
- Skin irritation (Category 2)
- Serious eye damage (Category 1)
- Carcinogenicity (Category 2)

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

Hazards statement:
- H301 Toxic if swallowed.
- H310 + H330 Fatal in contact with skin or inhaled.
- H315 Causes skin irritation.
- H318 Causes serious eye damage.
- H351 Suspected of causing cancer.

Precautionary statement:
- P260 Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P301 + P330 + 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.
- P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P310 Immediately call a POISON CENTER or doctor/ physician.

Section 3. Composition and information on ingredients

Name	CAS	Concentration %
Hexachloro-1,3-butadiene-$^{13}C_4$	93951-70-3	> 97

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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: 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: 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, hydrogen chloride 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: Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.
Environmental precautions: Do not let product enter drains.
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. 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) 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: 260.76 g/mol
Physical status: Liquid
Color: Colorless to light yellow
Odour: No data available
Density: 1.665 g/cm^3
Melting point: -21 °C (-6 °F)
Boiling point: 215 °C (419 °F)
Vapour density: 0.3 hPa (0.2 mmHg) at 20 °C (68 °F)
Vapour density: No data available
Partition coefficient (octanol/water): log Pow: 4.78
Solubility in water: 3.2 mg/L

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

Section 11. Toxicological information (unlabelled)

Toxicological data: Hexachloro-1,3-butadiene

Information on ingredients:

Name	CAS	LD_{50}	LC_{50}
Hexachloro-1,3-butadiene	87-68-3	Oral - Rat - 82 mg/kg Dermal - Rabbit - 100 mg/kg	Inhalation - Mouse - 370 mg/m^3

Potential acute effects

- **Eyes:** Causes serious eye damage.
- **Skin:** Fatal if absorbed through skin. Causes skin irritation.
- **Inhalation:** Fatal if inhaled. Causes respiratory tract irritation.
- **Ingestion:** Toxic if swallowed.

Potential chronic effects

- **Carcinogenic effects:** This product is or contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH, NTP, or EPA classification. Limited evidence of carcinogenicity in animal studies. IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Hexachlorobuta-1,3-diene).
- **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
Hexachloro-1,3-butadiene	0.14 mg/l EC50	Oncorhynchus mykiss	96 h

Effects on environment: No data available.
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: Contact a licensed professional waste disposal service to dispose of this material.

Section 14. Transportation information

Classification DOT/IMDG/IATA label:

Shipping name: Hexachlorobutadiene
UN number: UN2279
Class: 6.1
Packaging group: III

Additional information: None

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Section 15. Regulatory information

UNITED STATES:
NFPA classification

Health: 3
Flammable: 0
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: Hexachloro-1,3-butadiene
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

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.

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