Safety Data Sheet

Benzyl-2,3,4,5,6-d_5 Chloride

Section 1. Chemical product and company identifications

Product code: D-1652
Chemical formula: $C_7H_2D_5Cl$
CAS: 68661-11-0
CAS (unlabelled): 100-44-7
Synonyms: α-Chlorotoluene, (Chloromethyl)benzene, Tolyl Chloride

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: Liquid
Warning: Combustible liquid. Harmful if swallowed. Fatal if 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:
- Flammable liquids (Category 4)
- Acute toxicity, Oral (Category 4)
- Acute toxicity, Inhalation (Category 2)
- Skin irritation (Category 2)
- Serious eye damage (Category 1)
- Carcinogenicity (Category 1B)
- Specific target organ toxicity - single exposure (Category 3)
- Specific target organ toxicity - repeated exposure (Category 2)

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

Hazards statement:
- H227 Combustible liquid and vapour.
- H302 Harmful if swallowed.
- H315 Causes skin irritation.
- H318 Causes serious eye damage.
- H330 Fatal if inhaled.
- H335 May cause respiratory irritation.
- H350 May cause cancer.
- H371 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 + 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.

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Section 3. Composition and information on ingredients

Name	CAS	Concentration %
Benzyl-2,3,4,5,6-d_5 Chloride	68661-11-0	> 98

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: 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: 1.1 Vol%
Upper explosion limit: 14 Vol%
Auto-ignition temperature: 585 °C (1,085 °F)
Flash point: 67 °C (153 °F)
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: Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.
Environmental precautions: 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. Provide appropriate exhaust ventilation.
Storage: Store at room temperature. Adequate ventilation. Protect from heat and ignition sources. Protect from moisture.

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: 156.59 g/mol
Physical status: Liquid
Color: Colorless
Odour: Pungent
Density: 1.10 g/cm^3
Melting point: -43 °C (-45 °F)
Boiling point: 177 - 181 °C (351 - 358 °F)
Vapour pressure: 1.6 hPa (1.2 mmHg) at 25 °C (77 °F)
Vapour density: 4.37 (Air = 1)
Partition coefficient (octanol/water): log Pow: 2.3
Water solubility: 0.53 g/L

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Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.
Incompatibility: Bases, alcohols, amines, oxidizing agents.
Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides, hydrogen chloride gas.
Reactivity conditions: Heat, flames and sparks.

Section 11. Toxicological information (unlabelled)

Toxicological data: Benzyl Chloride

Information on ingredients:

Name	CAS	LD_{50}	LC_{50}
Benzyl Chloride	100-44-7	Oral - Rat - 1,231 mg/kg	Inhalation - Rat - 2 h - 0.74 mg/kg

Potential acute effects

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

Potential chronic effects

- **Carcinogenic effects:** 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: 2A - Group 2A: Probably carcinogenic to humans (Benzyl chloride).
- **Mutagenic effects:** Genotoxicity in vitro - S. typhimurium - with and without metabolic activation - This material has shown a positive Ames test, an in vitro test that indicates a possible potential to produce a carcinogenic effect. Genotoxicity in vivo - Mouse - Intraperitoneal – negative.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

Section 12. Ecological information

Ecological data:

Name	Results	Species	Period
Benzyl Chloride	4 mg/l LC50	Danio rerio	96 h
	6.1 mg/l EC50	Daphnia magna	48 h
	19.3 mg/l EC50	Pseudokirchneriella subcapitata	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: 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: Benzyl Chloride
UN number: UN1738
Class: 6.1 (8)
Packaging group: II

Additional information: None

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Section 15. Regulatory information

UNITED STATES:
NFPA classification

Health: 3
Flammable: 2
Reactivity: 1
Special conditions: None

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

U.S. Federal regulations:

TSCA 8(b) inventory: Benzyl Chloride
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: Listed
CWA (Clean Water Act) 311: 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):

B3 - Combustible liquid

D1A - Very toxic material causing immediate and serious toxic effects

D2A - Very toxic material causing other toxic effects
D2B - Toxic material causing other toxic effects

E - Corrosive material

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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