
1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Benzyl chloride- α -13C
Product Number : 288470
Brand : Aldrich
CAS-No. : 57742-41-3

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 Spruce Street
ST. LOUIS MO 63103
UNITED STATES
Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 4), H227

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Inhalation (Category 3), H331

Skin irritation (Category 2), H315

Serious eye damage (Category 1), H318

Carcinogenicity (Category 1B), H350

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

Specific target organ toxicity - repeated exposure (Category 2), H373

Acute aquatic toxicity (Category 2), H401

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Danger

Hazard statement(s)

H227	Combustible liquid.
H302	Harmful if swallowed.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H331	Toxic if inhaled.
H335	May cause respiratory irritation.
H350	May cause cancer.
H373	May cause damage to organs through prolonged or repeated exposure.
H401	Toxic to aquatic life.

Precautionary statement(s)

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P260	Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P281	Use personal protective equipment as required.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 + P311	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/ physician.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/doctor.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Lachrymator.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : α -Chlorotoluene- α -<SP>13</>C

Formula : $^{13}\text{C}_6\text{H}_7\text{Cl}$

Molecular weight : 127.57 g/mol

CAS-No. : 57742-41-3

Hazardous components

Component	Classification	Concentration
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Benzyl chloride-a-13C		
	Flam. Liq. 4; Acute Tox. 4; Acute Tox. 3; Skin Irrit. 2; Eye Dam. 1; Carc. 1B; STOT SE 3; STOT RE 2; Aquatic Acute 2; H227, H302, H315, H318, H331, H335, H350, H373, H401	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides, Hydrogen chloride gas

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations.

Vapours can accumulate in low areas.

For personal protection see section 8.

6.2 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.

6.3 Methods and materials for containment and 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.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

Storage class (TRGS 510): 6.1B: Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Benzyl chloride-a-13C	57742-41-3	TWA	1.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation Eye irritation Skin irritation Confirmed animal carcinogen with unknown relevance to humans		
		C	1.000000 ppm 5.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		15 minute ceiling value		
		TWA	1.000000 ppm 5.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		PEL	1 ppm 5 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

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) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: -43 °C (-45 °F) - lit.
f) Initial boiling point and boiling range	177 - 181 °C (351 - 358 °F) - lit.
g) Flash point	74 °C (165 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 14 %(V) Lower explosion limit: 1.1 %(V)
k) Vapour pressure	No data available
l) Vapour density	No data available
m) Relative density	1.109 g/cm ³ at 25 °C (77 °F)
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Auto-ignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Contact with common metals (except nickel and lead) or moisture produces a Friedel-Crafts, condensation-type reaction with the liberation of heat and formation of toxic and corrosive hydrogen chloride. Hydrolyzes very slowly to form hydrogen chloride and benzyl alcohol. This product is not sensitive to physical impact. When stabilized with propylene oxide, the possibility of a Friedel-Crafts type reaction is minimized. Depletion of the stabilizer increases the possibility of condensation reactions, Oxidizing agents, Iron and iron salts., Brass, Aluminum

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen chloride gas

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

Germ cell mutagenicity

No data available

Carcinogenicity

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-a-13C)

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

No data available

Specific target organ toxicity - single exposure

May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

The substance or mixture is classified as specific target organ toxicant, repeated exposure, category 2.

Aspiration hazard

Additional Information

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting

Stomach - Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence

12. ECOLOGICAL INFORMATION

12.1 Toxicity

No data available

12.2 Persistence and degradability

Biodegradability Biotic/Aerobic (Benzyl chloride-a-13C)
Result: 80 % - Readily biodegradable.

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available(Benzyl chloride-a-13C)

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Toxic to aquatic life.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

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. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 1738 Class: 6.1 (8) Packing group: II
Proper shipping name: Benzyl chloride
Reportable Quantity (RQ) : 100 lbs

Poison Inhalation Hazard: No

ALL INNER PACKAGINGS MUST BE IN METAL CANS FOR FXG

IMDG

UN number: 1738 Class: 6.1 (8) Packing group: II EMS-No: F-A, S-B
Proper shipping name: BENZYL CHLORIDE

IATA

UN number: 1738 Class: 6.1 (8) Packing group: II
Proper shipping name: Benzyl chloride
ALL INNER PACKAGINGS MUST BE IN METAL CANS FOR FX AIR

15. REGULATORY INFORMATION

SARA 302 Components

The following components are subject to reporting levels established by SARA Title III, Section 302:

	CAS-No.	Revision Date
Benzyl chloride-a-13C	57742-41-3	2007-07-01

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Benzyl chloride-a-13C	57742-41-3	2007-07-01

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Benzyl chloride-a-13C	57742-41-3	2007-07-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Benzyl chloride-a-13C	57742-41-3	2007-07-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Benzyl chloride-a-13C	57742-41-3	2007-07-01

California Prop. 65 Components

WARNING! This product contains a chemical known to the State of California to cause cancer.

	CAS-No.	Revision Date
Benzyl chloride-a-13C	57742-41-3	2007-09-28

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

H227	Combustible liquid.
H302	Harmful if swallowed.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H331	Toxic if inhaled.
H335	May cause respiratory irritation.
H350	May cause cancer.
H373	May cause damage to organs through prolonged or repeated exposure.
H401	Toxic to aquatic life.

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956
Version: 6.1

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