

## SAFETY DATA SHEET

Version 6.0  
Revision Date 09/28/2019  
Print Date 10/22/2019

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Benzyl bromide- $\alpha$ - $^{13}\text{C}$

Product Number : 488194  
Brand : Aldrich  
Index-No. : 602-057-00-2  
CAS-No. : 69838-86-4

**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

**SECTION 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  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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 : Warning

Hazard statement(s)  
H227 : Combustible liquid.

|                            |  |
|----------------------------|--|
| H315                       | Causes skin irritation.  |
| H319                       | Causes serious eye irritation.   |
| H335                       | May cause respiratory irritation.  |
| Precautionary statement(s) |  |
| P210                       | Keep away from heat/sparks/open flames/hot surfaces. No smoking.   |
| P261                       | Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.   |
| P264                       | Wash skin thoroughly after handling.   |
| P271                       | Use only outdoors or in a well-ventilated area.  |
| P280                       | Wear protective gloves/ protective clothing/ eye protection/ face protection.  |
| P302 + P352                | IF ON SKIN: Wash with plenty of soap and water.  |
| P304 + P340                | IF INHALED: Remove victim to fresh air and keep at rest in a position 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. |
| P312                       | Call a POISON CENTER/doctor if you feel unwell.  |
| P321                       | Specific treatment (see supplemental first aid instructions on this label).  |
| P332 + P313                | If skin irritation occurs: Get medical advice/ attention.  |
| P337 + P313                | If eye irritation persists: 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 - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |   |  |
|------------------|---|--|
| Synonyms         | : | $\alpha$ -Bromotoluene- $\alpha$ -13C<br>$\alpha$ -Bromotoluene- $\alpha$ -13C |
| Formula          | : | $^{13}\text{C}_6\text{H}_7\text{Br}$   |
| Molecular weight | : | 172.02 g/mol   |
| CAS-No.          | : | 69838-86-4   |
| Index-No.        | : | 602-057-00-2   |

| Component                                     | Classification  | Concentration |
|---|---|---------------|
| <b>Benzyl bromide-<math>\alpha</math>-13C</b> |   |               |
|   | Flam. Liq. 4; Skin Irrit. 2;<br>Eye Irrit. 2A; STOT SE 3;<br>H227, H315, H319, H335 | <= 100 %      |

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

---

## SECTION 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. 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

---

## SECTION 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 bromide 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.

---

## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. 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.

### **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.

---

## **SECTION 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): 10: Combustible liquids not in Storage Class 3

### **7.3 Specific end use(s)**

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

---

## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Components with workplace control parameters**

Contains no substances with occupational exposure limit values.

### **8.2 Exposure controls**

#### **Appropriate engineering controls**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### **Personal protective equipment**

##### **Eye/face protection**

Safety glasses with side-shields conforming to EN166 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**

Impervious clothing, 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.

---

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |   |   |
|---|---|
| a) Appearance                                   | Form: clear, liquid<br>Colour: light brown          |
| b) Odour  | unpleasant  |
| c) Odour Threshold                              | No data available                                   |
| d) pH   | No data available                                   |
| e) Melting point/freezing point                 | Melting point/range: -3 - -1 °C (27 - 30 °F) - lit. |
| f) Initial boiling point and boiling range      | 198 - 199 °C 388 - 390 °F - lit.                    |
| g) Flash point                                  | 86 °C (187 °F) - closed cup                         |
| h) Evaporation rate                             | No data available                                   |
| i) Flammability (solid, gas)                    | No data available                                   |
| j) Upper/lower flammability or explosive limits | No data available                                   |
| k) Vapour pressure                              | No data available                                   |
| l) Vapour density                               | No data available                                   |
| m) Relative density                             | 1.446 g/cm <sup>3</sup> 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

---

## **SECTION 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**

No data available

### **10.6 Hazardous decomposition products**

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

Other decomposition products - No data available

In the event of fire: see section 5

---

## **SECTION 11: Toxicological information**

### **11.1 Information on toxicological effects**

#### **Acute toxicity**

No data available

Inhalation: No data available

Dermal: No data available

#### **Skin corrosion/irritation**

No data available

#### **Serious eye damage/eye irritation**

#### **Respiratory or skin sensitisation**

No data available

#### **Germ cell mutagenicity**

#### **Carcinogenicity**

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.

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**

#### **Specific target organ toxicity - single exposure**

May cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

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

---

**SECTION 12: Ecological information****12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

No data available

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**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**

No data available

---

**SECTION 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.

---

**SECTION 14: Transport information****DOT (US)**

Aldrich - 488194

Page 7 of 9

UN number: 1737 Class: 6.1 (8) Packing group: II  
Proper shipping name: Benzyl bromide  
Poison Inhalation Hazard: No

**IMDG**

UN number: 1737 Class: 6.1 (8) Packing group: II EMS-No: F-A, S-B  
Proper shipping name: BENZYL BROMIDE

**IATA**

UN number: 1737 Class: 6.1 (8) Packing group: II  
Proper shipping name: Benzyl bromide

---

**SECTION 15: Regulatory information**

**SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

|                      | CAS-No.    | Revision Date |
|----------------------|------------|---------------|
| Benzyl bromide-a-13C | 69838-86-4 | 1993-04-24    |

**Pennsylvania Right To Know Components**

|                      | CAS-No.    | Revision Date |
|----------------------|------------|---------------|
| Benzyl bromide-a-13C | 69838-86-4 | 1993-04-24    |

**New Jersey Right To Know Components**

|                      | CAS-No.    | Revision Date |
|----------------------|------------|---------------|
| Benzyl bromide-a-13C | 69838-86-4 | 1993-04-24    |

**California Prop. 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

---

**SECTION 16: Other information**

**Further information**

Copyright 2018 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any



damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 6.0

Revision Date: 09/28/2019

Print Date: 10/22/2019