

# • SAFETY DATA SHEET

Version 6.6  
Revision Date 11/06/2025  
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## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : Bromobenzene-<sup>13</sup>C<sub>6</sub>  
Product Number : 488232  
Brand : Aldrich  
CAS-No. : 112630-77-0

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

Identified uses : Laboratory chemicals, Synthesis of substances  
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

### 1.3 Details of the supplier of the safety data sheet

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

### 1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

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## SECTION 2. HAZARDS IDENTIFICATION

**GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)**

**Hazards for the product as supplied**

Flammable liquids : Category 3

Skin irritation : Category 2  
Short-term (acute) aquatic hazard : Category 2  
Long-term (chronic) aquatic hazard : Category 2

### Other hazards

None known.

### GHS label elements

Hazard pictograms : 

Signal word : Warning

Hazard statements : H226 Flammable liquid and vapour.  
H315 Causes skin irritation.  
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**  
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.  
P233 Keep container tightly closed.  
P240 Ground/bond container and receiving equipment.  
P241 Use explosion-proof electrical/ ventilating/ lighting equipment.  
P242 Use only non-sparking tools.  
P243 Take precautionary measures against static discharge.  
P264 Wash skin thoroughly after handling.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/ eye protection/ face protection.  
**Response:**  
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.  
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 to extinguish.  
P391 Collect spillage.  
**Storage:**  
P403 + P235 Store in a well-ventilated place. Keep cool.

**Disposal:**

P501 Dispose of contents/ container to an approved waste disposal plant.

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**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Substance / Mixture : Substance  
CAS-No. : 112630-77-0

**Components**

| Chemical name     | CAS No./Unique ID | Concentration (% w/w) | Trade secret |
|-------------------|-------------------|-----------------------|--------------|
| Bromobenzene-13C6 | 112630-77-0*      | >= 90 - <= 100        | -            |

\* Indicates that the identifier is a CAS No.  
Actual concentration is withheld as a trade secret

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**SECTION 4. FIRST AID MEASURES**

General advice : Show this safety data sheet to the doctor in attendance.  
If inhaled : After inhalation: fresh air.  
In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.  
In case of eye contact : After eye contact: rinse out with plenty of water. Remove contact lenses.  
If swallowed : After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.  
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  
Protection of first-aiders : For personal protection see section 8.  
Notes to physician : No data available

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**SECTION 5. FIREFIGHTING MEASURES**

Suitable extinguishing media : Water  
Foam  
Carbon dioxide (CO<sub>2</sub>)

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Dry powder

Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting : Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products : Carbon oxides

Hydrogen bromide gas

Specific extinguishing methods : No data available

Further information : Remove container from danger zone and cool with water.  
Suppress (knock down) gases/vapours/mists with a water spray jet.  
Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:  
Do not breathe vapours, aerosols.  
Avoid substance contact.  
Ensure adequate ventilation.  
Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

For personal protection see section 8.

Environmental precautions : Do not let product enter drains.  
Risk of explosion.

Methods and materials for containment and cleaning up : Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10).  
Take up with liquid-absorbent material (e.g. Chemizorb® ). Dispose of properly. Clean up affected area.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion : Keep away from open flames, hot surfaces and sources of ignition.  
Take precautionary measures against static discharge.

Further information on storage conditions : Keep container tightly closed in a dry and well-ventilated place.  
Keep away from heat and sources of ignition.

Storage class : 3, Flammable liquids

Recommended storage temperature : Recommended storage temperature see product label.

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.  
Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter A-(P2)

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The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Material : Viton®  
Break through time : 480 min  
Glove thickness : 0.7 mm  
Protective index : Full contact  
Manufacturer : Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Material : butyl-rubber  
Break through time : 30 min  
Glove thickness : 0.7 mm  
Protective index : Splash contact  
Manufacturer : Butoject® (KCL 898)

Remarks : This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  
Safety glasses

Skin and body protection : Flame retardant antistatic protective clothing.

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid  
Color : colourless  
Odor : No data available

|   |   |
|---|---|
| Odor Threshold                                      | : No data available                       |
| pH  | : No data available                       |
| Melting point                                       | : -24 °F / -31 °C                         |
| Boiling point                                       | : 313 °F / 156 °C                         |
| Flash point   | : 124 °F / 51 °C                          |
|   | Method: closed cup                        |
| Evaporation rate                                    | : No data available                       |
| Flammability (solid, gas)                           | : No data available                       |
| Flammability (liquids)                              | : No data available                       |
| Burning rate  | : No data available                       |
| Upper explosion limit /<br>Upper flammability limit | : 36.5 %(V)                               |
| Lower explosion limit /<br>Lower flammability limit | : 6 %(V)                                  |
| Vapor pressure                                      | : No data available                       |
| Relative vapour density                             | : No data available                       |
| Relative density                                    | : No data available                       |
| Density   | : 1.547 g/cm <sup>3</sup> (77 °F / 25 °C) |
| Water solubility                                    | : No data available                       |
| Partition coefficient: n-<br>octanol/water          | : No data available                       |
| Autoignition temperature                            | : No data available                       |
| Decomposition<br>temperature                        | : No data available                       |
| Viscosity, dynamic                                  | : No data available                       |
| Viscosity, kinematic                                | : No data available                       |
| Flow time   | : No data available                       |
| Explosive properties                                | : No data available                       |

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**MILLIPORE  
SIGMA**

Oxidizing properties : none  
Molecular weight : 162.90 g/mol  
Particle characteristics  
Particle size : No data available

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## SECTION 10. STABILITY AND REACTIVITY

Reactivity : Vapour/air-mixtures are explosive at intense warming.  
Chemical stability : The product is chemically stable under standard ambient conditions (room temperature) .  
Possibility of hazardous reactions : Violent reactions possible with:  
Oxidizing agents  
peroxi compounds  
Alkali metals  
Alkaline earth metals  
Conditions to avoid : Heating.  
Incompatible materials : No data available  
Hazardous decomposition products : In the event of fire: see section 5

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## SECTION 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male - 2,383 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: bromobenzene

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract., Aspiration may cause pulmonary oedema and pneumonitis.

LC50 Inhalation - Rat - 20.4 mg/l - vapour

Remarks: (RTECS)

The value is given in analogy to the following substances: bromobenzene

Symptoms: Inhalation may lead to the formation of oedemas in the respiratory tract.

Dermal: No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 4 h

(OECD Test Guideline 404)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

The value is given in analogy to the following substances: bromobenzene

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

Eyes - Rabbit

Result: No eye irritation - 24 h

(OECD Test Guideline 405)

Remarks: The value is given in analogy to the following substances: bromobenzene

### **Respiratory or skin sensitization**

No data available

### **Germ cell mutagenicity**

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances:  
bromobenzene

### **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**

No data available

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

No data available

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

No data available

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

Liver injury may occur., Kidney injury may occur., Vomiting, Diarrhoea, Abdominal pain  
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption of large quantities:

Systemic effects:

Headache  
Vomiting  
Diarrhoea  
agitation  
narcosis

Absorption can result in damage to:

Liver

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Kidney

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12. ECOLOGICAL INFORMATION

### Ecotoxicity

#### Components:

##### **Bromobenzene-13C6:**

- Toxicity to fish : LC50 (Pimephales promelas (fathead minnow)): 5.6 mg/l  
Exposure time: 96 h  
Remarks: (ECOTOX Database)  
The value is given in analogy to the following substances:  
The value is given in analogy to the following substances: bromobenzene
- Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 15.7 mg/l  
End point: Immobilization  
Exposure time: 48 h  
Method: OECD Test Guideline 202  
Remarks: The value is given in analogy to the following substances:  
The value is given in analogy to the following substances: bromobenzene
- Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata): 12.3 mg/l  
Exposure time: 72 h  
Test Type: static test  
Analytical monitoring: yes  
GLP: yes  
Remarks: (ECHA)  
The value is given in analogy to the following substances:  
The value is given in analogy to the following substances: bromobenzene
- NOEC (Pseudokirchneriella subcapitata): 4.87 mg/l  
Exposure time: 72 h  
Test Type: static test  
Analytical monitoring: yes  
GLP: yes  
Remarks: (ECHA)  
The value is given in analogy to the following substances:  
The value is given in analogy to the following

substances: bromobenzene

### **Persistence and degradability**

#### **Components:**

##### **Bromobenzene-13C6:**

Biodegradability : aerobic  
Inoculum: activated sludge  
Result: Not readily biodegradable.  
Biodegradation: 0 %  
Exposure time: 28 d  
Remarks: (HSDB)  
The value is given in analogy to the following substances:  
The value is given in analogy to the following substances: bromobenzene

### **Bioaccumulative potential**

#### **Components:**

##### **Bromobenzene-13C6:**

Bioaccumulation : Remarks: No data available

### **Mobility in soil**

#### **Components:**

##### **Bromobenzene-13C6:**

Stability in soil : Remarks: No data available

### **Other adverse effects**

#### **Components:**

##### **Bromobenzene-13C6:**

Additional ecological information : Discharge into the environment must be avoided.  
The value is given in analogy to the following substances: bromobenzene

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## **SECTION 13. DISPOSAL CONSIDERATIONS**

### **Disposal methods**

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14. TRANSPORT INFORMATION

### International Regulations

#### IATA-DGR

UN/ID No. : UN 2514  
Proper shipping name : Bromobenzene  
Class : 3  
Packing group : III  
Labels : Class 3 - Flammable liquids  
Packing instruction (cargo aircraft) : 366  
Packing instruction (passenger aircraft) : 355

#### IMDG-Code

UN number : UN 2514  
Proper shipping name : BROMOBENZENE  
  
Class : 3  
Packing group : III  
Labels : 3  
EmS Code : F-E, S-D  
Marine pollutant : yes

#### Transport in bulk according to IMO instruments

Not applicable for product as supplied.

### National Regulations

#### 49 CFR Road

UN/ID/NA number : UN 2514  
Proper shipping name : Bromobenzene  
  
Class : 3  
Packing group : III  
Labels : Class 3 - Flammable liquids  
ERG Code : 130  
Marine pollutant : yes  
  
Poison Inhalation Hazard : No

#### Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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## SECTION 15. REGULATORY INFORMATION

#### CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

### **SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

### **SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Fire Hazard  
Acute Health Hazard

**SARA 313** : 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.

### **US State Regulations**

#### **Massachusetts Right To Know**

Bromobenzene-13C6 112630-77-0

#### **Pennsylvania Right To Know**

Bromobenzene-13C6 112630-77-0

#### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

### **The components of this product are reported in the following inventories:**

TSCA : Product contains substance(s) not listed on TSCA inventory.

#### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16. OTHER INFORMATION**

### **Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response;

EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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