

Safety Data Sheet

acc. to OSHA HCS

Printing date 05/10/2020

Revision date 05/10/2020

1 Identification

- **Product identifier**
- **Trade name:** **Bromobenzene-13C6**
- **Synonym** 1-bromo-benzene-1,2,3,4,5,6-13C6
- **Article number:** 30524
- **CAS Number:**
112630-77-0
- **EC number:**
625-398-9
- **Application of the substance / the mixture** For research use only - not for human or veterinary use.
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**
Cayman Chemical Co.
1180 E. Ellsworth Rd.
Ann Arbor, MI 48108
USA
- **Information department:** Product safety department
- **Emergency telephone number:**
During normal opening times: +1 (734) 971-3335
US/CANADA: 800-424-9300
Outside US/CANADA: 703-741-5970

2 Hazard(s) identification

- **Classification of the substance or mixture**



GHS02 Flame

Flam. Liq. 3 H226 Flammable liquid and vapor.



GHS09 Environment

Aquatic Chronic 2 H411 Toxic to aquatic life with long lasting effects.



GHS07

Skin Irrit. 2 H315 Causes skin irritation.

- **Label elements**

- **GHS label elements**

The substance is classified and labeled according to the Globally Harmonized System (GHS).

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Hazard pictograms



GHS02 GHS07 GHS09

Signal word Warning

Hazard statements

Flammable liquid and vapor.
Causes skin irritation.
Toxic to aquatic life with long lasting effects.

Precautionary statements

Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
Keep container tightly closed.
Ground/bond container and receiving equipment.
Use explosion-proof electrical/ventilating/lighting/equipment.
Use only non-sparking tools.
Take precautionary measures against static discharge.
Wash thoroughly after handling.
Avoid release to the environment.
Wear protective gloves/protective clothing/eye protection/face protection.
Specific treatment (see on this label).
If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
If skin irritation occurs: Get medical advice/attention.
Take off contaminated clothing and wash it before reuse.
In case of fire: Use for extinction: CO₂, powder or water spray.
Collect spillage.
Store in a well-ventilated place. Keep cool.
Dispose of contents/container in accordance with local/regional/national/international regulations.

Classification system:

NFPA ratings (scale 0 - 4)



Health = 1
Fire = 2
Reactivity = 0

HMIS-ratings (scale 0 - 4)



Health = 1
Fire = 2
Reactivity = 0

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.
vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances

CAS No. Description

112630-77-0 Bromobenzene-13C6

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- **Identification number(s)**
- **EC number:** 625-398-9

4 First-aid measures

- **Description of first aid measures**
- **After inhalation:** In case of unconsciousness place patient stably in side position for transportation.
- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
- **After eye contact:** Rinse opened eye for several minutes under running water.
- **After swallowing:** If symptoms persist consult doctor.
- **Information for doctor:**
- **Most important symptoms and effects, both acute and delayed**
May cause anemia, cough, CNS depression, drowsiness, headache, heart damage, lassitude (weakness, exhaustion), liver damage, narcosis, reproductive effects, teratogenic effects.
No further relevant information available.
- **Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

5 Fire-fighting measures

- **Extinguishing media**
- **Suitable extinguishing agents:**
CO2, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **Special hazards arising from the substance or mixture** No further relevant information available.
- **Advice for firefighters**
- **Protective equipment:** No special measures required.

6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures**
Wear protective equipment. Keep unprotected persons away.
- **Environmental precautions:**
Inform respective authorities in case of seepage into water course or sewage system.
Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:**
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Ensure adequate ventilation.
- **Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.
- **Protective Action Criteria for Chemicals**
- **PAC-1:** Substance is not listed.
- **PAC-2:** Substance is not listed.
- **PAC-3:** Substance is not listed.

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7 Handling and storage

- **Handling:**
- **Precautions for safe handling**
No special precautions are necessary if used correctly.
Avoid breathing dust/fume/gas/mist/vapours/spray.
Avoid prolonged or repeated exposure.
Keep away from sources of ignition.
Take precautionary measures against static discharge.re.
- **Information about protection against explosions and fires:**
Keep ignition sources away - Do not smoke.
Protect against electrostatic charges.
- **Conditions for safe storage, including any incompatibilities**
Keep container tightly closed.
Store in accordance with information listed on the product insert.
- **Storage:**
- **Requirements to be met by storerooms and receptacles:** No special requirements.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:** Keep receptacle tightly sealed.
- **Specific end use(s)** No further relevant information available.

8 Exposure controls/personal protection

- **Additional information about design of technical systems:** No further data; see item 7.
- **Control parameters**
- **Components with limit values that require monitoring at the workplace:** Not required.
- **Additional information:** The lists that were valid during the creation were used as basis.
- **Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:**
Keep away from foodstuffs, beverages and feed.
Immediately remove all soiled and contaminated clothing.
Wash hands before breaks and at the end of work.
Avoid contact with the skin.
Avoid contact with the eyes and skin.
- **Breathing equipment:** Not required.
- **Protection of hands:**



Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.
Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

- **Material of gloves**

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

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- **Penetration time of glove material**

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

- **Eye protection:**



Tightly sealed goggles

9 Physical and chemical properties

- **Information on basic physical and chemical properties**

- **General Information**

- **Appearance:**

- Form:

Liquid

- Color:

Not determined.

- **Odor:**

Characteristic

- **Structural Formula**

[13C]6H5Br

- **Molecular Weight**

163

- **Odor threshold:**

Not determined.

- **pH-value:**

Not determined.

- **Change in condition**

- Melting point/Melting range:

Undetermined.

- Boiling point/Boiling range:

156 °C (312.8 °F)

- **Flash point:**

51 °C (123.8 °F)

- **Flammability (solid, gaseous):**

Not applicable.

- **Decomposition temperature:**

Not determined.

- **Auto igniting:**

Not determined.

- **Danger of explosion:**

Product is not explosive. However, formation of explosive air/vapor mixtures are possible.

- **Explosion limits:**

- Lower:

Not determined.

- Upper:

Not determined.

- **Vapor pressure:**

Not determined.

- **Density:**

Not determined.

- **Relative density**

Not determined.

- **Vapor density**

Not determined.

- **Evaporation rate**

Not determined.

- **Solubility in / Miscibility with**

- Water:

Not determined.

- **Partition coefficient (n-octanol/water):** Not determined.

- **Viscosity:**

- Dynamic:

Not determined.

- Kinematic:

Not determined.

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SOLUBILITY

~0.2 mg/ml in a 1:4 solution of EtOH:PBS (pH 7.2); ~30 mg/ml in EtOH; DMSO; DMF

· **Other information**

No further relevant information available.

10 Stability and reactivity

- **Reactivity** No further relevant information available.
- **Chemical stability**
- **Thermal decomposition / conditions to be avoided:**
No decomposition if used according to specifications.
- **Possibility of hazardous reactions** No dangerous reactions known.
- **Conditions to avoid** No further relevant information available.
- **Incompatible materials:** strong oxidizing agents
- **Hazardous decomposition products:** carbon oxides, hydrogen bromide

11 Toxicological information

- **Information on toxicological effects**
- **Acute toxicity:**
- **Primary irritant effect:**
- **on the skin:** Irritant to skin and mucous membranes.
- **on the eye:** No irritating effect.
- **Sensitization:** No sensitizing effects known.
- **Additional toxicological information:**
- **Carcinogenic categories**
- **IARC (International Agency for Research on Cancer)** Substance is not listed.
- **NTP (National Toxicology Program)** Substance is not listed.
- **OSHA-Ca (Occupational Safety & Health Administration)** Substance is not listed.

12 Ecological information

- **Toxicity**
- **Aquatic toxicity:** No further relevant information available.
- **Persistence and degradability** No further relevant information available.
- **Behavior in environmental systems:**
- **Bioaccumulative potential** No further relevant information available.
- **Mobility in soil** No further relevant information available.
- **Ecotoxicological effects:**
- **Remark:** Toxic for fish
- **Additional ecological information:**
- **General notes:**
Water hazard class 2 (Self-assessment): hazardous for water
Do not allow product to reach ground water, water course or sewage system.
Danger to drinking water if even small quantities leak into the ground.
Also poisonous for fish and plankton in water bodies.
Toxic for aquatic organisms
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.

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- **Other adverse effects** No further relevant information available.

13 Disposal considerations

- **Waste treatment methods**
- **Recommendation:**
Must not be disposed of together with household garbage. Do not allow product to reach sewage system.
- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.

14 Transport information

- | | |
|---|---|
| · UN-Number | UN2514 |
| · DOT, IMDG, IATA | |
| · UN proper shipping name | Bromobenzene |
| · DOT, IATA | BROMOBENZENE, MARINE POLLUTANT |
| · IMDG | |
| · Transport hazard class(es) | |
| · DOT | |
|   | |
| · Class | 3 Flammable liquids |
| · Label | 3 |
| · IMDG | |
|   | |
| · Class | 3 Flammable liquids |
| · Label | 3 |
| · IATA | |
|  | |
| · Class | 3 Flammable liquids |
| · Label | 3 |
| · Packing group | III |
| · DOT, IMDG, IATA | |
| · Environmental hazards: | Environmentally hazardous substance, liquid; Marine Pollutant |

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· Marine pollutant:	Yes (DOT) Symbol (fish and tree)
· Special precautions for user	Warning: Flammable liquids
· Hazard identification number (Kemler code):	30
· EMS Number:	F-E,S-D
· Stowage Category	A
· Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
· Transport/Additional information:	
· DOT	
· Quantity limitations	On passenger aircraft/rail: 60 L On cargo aircraft only: 220 L
· Remarks:	Special marking with the symbol (fish and tree).
· IMDG	
· Limited quantities (LQ)	5L
· Excepted quantities (EQ)	Code: E1 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 1000 ml
· IATA	
· Remarks:	When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.
· UN "Model Regulation":	UN 2514 BROMOBENZENE, 3, III, ENVIRONMENTALLY HAZARDOUS

15 Regulatory information

- Safety, health and environmental regulations/legislation specific for the substance or mixture
 - Sara
 - Section 355 (extremely hazardous substances): Substance is not listed.
 - Section 313 (Specific toxic chemical listings): Substance is not listed.
 - TSCA (Toxic Substances Control Act): Substance is not listed.
 - Hazardous Air Pollutants Substance is not listed.
 - Proposition 65
 - Chemicals known to cause cancer: Substance is not listed.
 - Chemicals known to cause reproductive toxicity for females: Substance is not listed.
 - Chemicals known to cause reproductive toxicity for males: Substance is not listed.
 - Chemicals known to cause developmental toxicity: Substance is not listed.
 - Carcinogenic categories
 - EPA (Environmental Protection Agency) Substance is not listed.
 - TLV (Threshold Limit Value established by ACGIH) Substance is not listed.
 - NIOSH-Ca (National Institute for Occupational Safety and Health) Substance is not listed.
 - GHS label elements
- The substance is classified and labeled according to the Globally Harmonized System (GHS).

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· Hazard pictograms



GHS02 GHS07 GHS09

· Signal word Warning

· Hazard statements

Flammable liquid and vapor.

Causes skin irritation.

Toxic to aquatic life with long lasting effects.

· Precautionary statements

Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

Keep container tightly closed.

Ground/bond container and receiving equipment.

Use explosion-proof electrical/ventilating/lighting/equipment.

Use only non-sparking tools.

Take precautionary measures against static discharge.

Wash thoroughly after handling.

Avoid release to the environment.

Wear protective gloves/protective clothing/eye protection/face protection.

Specific treatment (see on this label).

If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

If skin irritation occurs: Get medical advice/attention.

Take off contaminated clothing and wash it before reuse.

In case of fire: Use for extinction: CO2, powder or water spray.

Collect spillage.

Store in a well-ventilated place. Keep cool.

Dispose of contents/container in accordance with local/regional/national/international regulations.

· Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

· Department issuing SDS: Environment protection department.

· Contact: -

· Date of preparation / last revision 05/10/2020 / -

· Abbreviations and acronyms:

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

ACGIH: American Conference of Governmental Industrial Hygienists

EINECS: European Inventory of Existing Commercial Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMIS: Hazardous Materials Identification System (USA)

PBT: Persistent, Bioaccumulative and Toxic

vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

Flam. Liq. 3: Flammable liquids – Category 3

Skin Irrit. 2: Skin corrosion/irritation – Category 2

Aquatic Chronic 2: Hazardous to the aquatic environment - long-term aquatic hazard – Category 2