

SAFETY DATA SHEET

Version 6.4
Revision Date 10/27/2023
Print Date 02/24/2024

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

Product name : Bromobenzene-d₅
Product Number : 175730
Brand : Aldrich
CAS-No. : 4165-57-5

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 ST
ST. LOUIS MO 63103
UNITED STATES
Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

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

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 3), H226
Skin irritation (Category 2), H315
Short-term (acute) aquatic hazard (Category 2), H401
Long-term (chronic) aquatic hazard (Category 2), H411

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)	
H226	Flammable liquid and vapor.
H315	Causes skin irritation.
H411	Toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
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.
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.
P403 + P235	Store in a well-ventilated place. Keep cool.
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	: Pentadeuterobromobenzene
Formula	: C ₆ BrD ₅
Molecular weight	: 162.06 g/mol
CAS-No.	: 4165-57-5
EC-No.	: 224-013-8

Component	Classification	Concentration
bromobenzene-d₅		
	Flam. Liq. 3; Skin Irrit. 2; Aquatic Acute 2; Aquatic Chronic 2; H226, H315, H401, H411	<= 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

Show this material 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.

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

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Hydrogen bromide gas

Combustible.

Vapors 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.

5.3 Advice for firefighters

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

5.4 Further information

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

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, 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. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 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.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

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

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

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

Personal protective equipment

Eye/face protection

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

Skin protection

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).

Full contact

Material: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

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).

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 30 min

Material tested: Butoject® (KCL 898)

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter A-(P2)

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.

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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: clear, liquid Color: colorless
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	156 °C 313 °F
g) Flash point	51 °C (124 °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: 2.5 %(V) Lower explosion limit: 0.5 %(V)
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	1.539 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents

peroxi compounds

Alkali metals

Alkaline earth metals

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

In the event of fire: see section 5

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 edema and pneumonitis.

LC50 Inhalation - Rat - 20.4 mg/l - vapor

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

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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 ingredient 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 ingredient 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, Diarrhea, 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

Diarrhea

agitation

narcosis

Absorption can result in damage to:

Liver

Kidney

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

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SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 5.6 mg/l - 96 h Remarks: (ECOTOX Database) 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 - 48 h (OECD Test Guideline 202) Remarks: The value is given in analogy to the following substances: bromobenzene
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - 12.3 mg/l - 72 h Remarks: (ECHA) The value is given in analogy to the following substances: bromobenzene static test NOEC - Pseudokirchneriella subcapitata - 4.87 mg/l - 72 h Remarks: (ECHA) The value is given in analogy to the following substances: bromobenzene

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 0 % - Not readily biodegradable. Remarks: (HSDB) The value is given in analogy to the following substances: bromobenzene
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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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

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.

SECTION 14: Transport information

DOT (US)

UN number: 2514 Class: 3 Packing group: III
Proper shipping name: Bromobenzene
Reportable Quantity (RQ):
Marine pollutant: yes Poison Inhalation Hazard: No

IMDG

UN number: 2514 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: BROMOBENZENE
Marine pollutant : yes
Marine pollutant : yes

IATA

UN number: 2514 Class: 3 Packing group: III
Proper shipping name: Bromobenzene

SECTION 15: Regulatory information

SARA 302 Components

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

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.

Massachusetts Right To Know Components

bromobenzene-d ₅	CAS-No. 4165-57-5	Revision Date 1993-04-24
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Pennsylvania Right To Know Components

bromobenzene-d ₅	CAS-No. 4165-57-5	Revision Date 1993-04-24
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SECTION 16: Other information

Further information

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Details in analogy to the undeuterated compound.
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