

SAFETY DATA SHEET

Version 8.9
Revision Date 03/08/2024
Print Date 05/12/2024**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 1-Bromobutane for synthesis

Product Number : 8.01602
Catalogue No. : 801602
Brand : Millipore
CAS-No. : 109-65-9

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

Identified uses : Chemical for synthesis
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

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 2), H225
Skin irritation (Category 2), H315
Carcinogenicity (Category 2), H351
Reproductive toxicity (Category 1B), H360

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Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Specific target organ toxicity - repeated exposure, Inhalation (Category 2), Liver, H373
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

Danger

Hazard Statements

H225 Highly flammable liquid and vapor.
H315 Causes skin irritation.
H335 May cause respiratory irritation.
H351 Suspected of causing cancer.
H360 May damage fertility or the unborn child.
H373 May cause damage to organs (Liver) through prolonged or repeated exposure if inhaled.
H411 Toxic to aquatic life with long lasting effects.

Precautionary Statements

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.
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.
P260 Do not breathe mist or vapors.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
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 to extinguish.
P391 Collect spillage.
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.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none**SECTION 3: Composition/information on ingredients****3.1 Substances**

Formula	: C ₄ H ₉ Br
Molecular weight	: 137.03 g/mol
CAS-No.	: 109-65-9
EC-No.	: 203-691-9

Component	Classification	Concentration
1-bromobutane		
	Flam. Liq. 2; Skin Irrit. 2; Carc. 2; Repr. 1B; STOT SE 3; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H225, H315, H351, H360, H335, H373, 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. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

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.

Fire may cause evolution of:

hydrogen bromide

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

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

Forms explosive mixtures with air at ambient temperatures.

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 carefully 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 safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

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

Protected from light. Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Recommended storage temperature see product label.

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: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 60 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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: liquid
Color: colorless |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: -112 °C (-170 °F) |
| f) Initial boiling point and boiling range | 99 - 101 °C 210 - 214 °F at 1,013 hPa |
| g) Flash point | 10 °C (50 °F) - closed cup |

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h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 6.6 %(V) Lower explosion limit: 2.8 %(V)
k)	Vapor pressure	200 hPa at 50 °C (122 °F) 53 hPa at 25 °C(77 °F)
l)	Vapor density	4.73 - (Air = 1.0)
m)	Density	1.273 g/cm ³ at 25 °C (77 °F)
	Relative density	No data available
n)	Water solubility	0.869 g/l at 25 °C (77 °F) - partly soluble
o)	Partition coefficient: n-octanol/water	log Pow: 2.75 - Bioaccumulation is not expected., (ECHA)
p)	Autoignition temperature	265 °C (509 °F)
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

Surface tension	25.9 mN/m at 25 °C (77 °F)
Relative vapor density	4.73 - (Air = 1.0)

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

peroxi compounds
Alkali metals
Alkaline earth metals
Powdered metals
Strong oxidizing agents
fats
various plastics
Exothermic reaction with:

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10.4 Conditions to avoid

Warming.

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

Acute toxicity estimate Oral - 2,817 mg/kg

(Calculation method)

LD50 Oral - Rat - 2,761 mg/kg (1-bromobutane)

Remarks: Behavioral:Somnolence (general depressed activity).

Behavioral:Tremor.

Behavioral:Ataxia.

(RTECS)

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract, Headache, inebriation, Dizziness, Unconsciousness

Acute toxicity estimate Dermal - 2,551 mg/kg

(Calculation method)

LD50 Dermal - Rat - male and female - > 2,000 mg/kg (1-bromobutane)

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit (1-bromobutane)

Result: Irritating to skin.

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit (1-bromobutane)

Result: No eye irritation - 1 s

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig (1-bromobutane)

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

(1-bromobutane)

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: In vitro mammalian cell gene mutation test

(1-bromobutane)

Test system: mouse lymphoma cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: positive
(1-bromobutane)
Test Type: Micronucleus test
Species: Mouse
Cell type: Red blood cells (erythrocytes)
Application Route: Intraperitoneal
Method: OECD Test Guideline 474
Result: negative

Carcinogenicity

Suspected of causing cancer. (1-bromobutane)

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

May damage fertility. (1-bromobutane)

May damage the unborn child. (1-bromobutane)

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. (1-bromobutane)

Specific target organ toxicity - repeated exposure

Inhalation - May cause damage to organs through prolonged or repeated exposure.

- Liver

Aspiration hazard

No data available

11.2 Additional Information

Cough, Shortness of breath, Headache, Nausea, Vomiting (1-bromobutane)

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (1-bromobutane)

Chronic intoxication:

(1-bromobutane)

Damage to:

(1-bromobutane)

Liver

(1-bromobutane)

Other dangerous properties can not be excluded.

(1-bromobutane)

Handle in accordance with good industrial hygiene and safety practice.

(1-bromobutane)

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - 24.3 mg/l - 96 h (1-bromobutane) (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 99.3 mg/l - 48 h (1-bromobutane) (OECD Test Guideline 202)
Toxicity to algae	ErC50 - Pseudokirchneriella subcapitata (green algae) - 9.98 mg/l - 72 h (1-bromobutane) (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - activated sludge - 270 mg/l - 5 min (1-bromobutane) Remarks: (ECHA)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d (1-bromobutane) Result: 19.2 % - Not readily biodegradable. (OECD Test Guideline 301D)
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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: 1126 Class: 3 Packing group: II
Proper shipping name: 1-Bromobutane
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 1126 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: 1-BROMOBUTANE
Marine pollutant : yes

IATA

UN number: 1126 Class: 3 Packing group: II
Proper shipping name: 1-Bromobutane

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

	CAS-No.	Revision Date
1-bromobutane	109-65-9	2007-03-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
1-bromobutane	109-65-9	2007-03-01

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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