

SAFETY DATA SHEET

Version 8.10
Revision Date 09/07/2024
Print Date 09/08/2024**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 1-Chlorobutane for synthesis

Product Number : 8.01640
Catalogue No. : 801640
Brand : Millipore
Index-No. : 602-059-00-3
CAS-No. : 109-69-3

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
Aspiration hazard (Category 1), H304
Short-term (acute) aquatic hazard (Category 3), H402

Long-term (chronic) aquatic hazard (Category 3), H412

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.

H304

May be fatal if swallowed and enters airways.

H412

Harmful to aquatic life with long lasting effects.

Precautionary Statements

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.

P273

Avoid release to the environment.

P280

Wear protective gloves/ eye protection/ face protection.

P301 + P310

IF SWALLOWED: Immediately call a POISON CENTER/ doctor.

P303 + P361 + P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

P331

Do NOT induce vomiting.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

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

| | |
|------------------|----------------|
| Formula | : C4H9Cl |
| Molecular weight | : 92.57 g/mol |
| CAS-No. | : 109-69-3 |
| EC-No. | : 203-696-6 |
| Index-No. | : 602-059-00-3 |

| Component | Classification | Concentration |
|-----------------------|--|---------------|
| 1-chlorobutane | Flam. Liq. 2; Asp. Tox. 1; Aquatic Acute 3; Aquatic Chronic 3; H225, H304, | <= 100 % |

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**MILLIPORE
SIGMA**

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: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

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

Carbon dioxide (CO₂) Foam 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 chloride gas

Combustible.

Fire may cause evolution of:

Hydrogen chloride gas, Phosgene

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

In the event of fire, wear self-contained breathing apparatus.

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 protection against fire and explosion

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

Hygiene measures

Change contaminated clothing. Wash hands 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.

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

Change contaminated clothing. Wash hands 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: 10 min

Material tested: Butoject® (KCL 898)

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 | stinging |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/ range: -123.1 °C (-189.6 °F) at ca.1,013.25 hPa |
| f) Initial boiling point and boiling range | 77 - 78 °C 171 - 172 °F at 1,013 hPa |
| g) Flash point | -12 °C (10 °F) at ca.1,013.25 hPa - closed cup - Regulation (EC) No. 440/2008, Annex, A.9 |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 10.1 %(V) Lower explosion limit: 1.8 %(V) |
| k) Vapor pressure | 120.6 hPa at 20 °C (68 °F) - OECD Test Guideline 104 |
| l) Vapor density | 3.2 - (Air = 1.0) |
| m) Density | 0.886 g/cm ³ at 20 °C (68 °F) |
| Relative density | 0.8820 °C |
| n) Water solubility | ca.0.11 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - partly soluble |
| o) Partition coefficient: n-octanol/water | log Pow: 2.66 at 20 °C (68 °F) - OECD Test Guideline 107 - Bioaccumulation is not expected. |
| p) Autoignition temperature | 245 °C (473 °F) at 1,013.25 hPa |
| 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 63.2 mN/m at 0.1g/l at 20 °C (68 °F) - OECD Test Guideline 115

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Relative vapor density 3.2 - (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

Risk of explosion with:

Alkali metals

Alkaline earth metals

sodium amide

Risk of ignition or formation of inflammable gases or vapours with:

Oxidizing agents

Powdered light metals

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

various plastics, Light metals

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 - 2,200 mg/kg

Remarks: (RTECS)

LC50 Inhalation - Rat - male and female - 4 h - > 7.74 mg/l - aerosol

(OECD Test Guideline 403)

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Micronucleus test

Species: Mouse

Cell type: Bone marrow

Application Route: Intraperitoneal

Method: OECD Test Guideline 474

Result: negative

Carcinogenicity

Animal testing did not show any carcinogenic effects.

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 toxicity to reproduction

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

May be fatal if swallowed and enters airways.

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 90 Days - NOAEL (No observed adverse effect level) - 120 mg/kg - LOAEL (Lowest observed adverse effect level) - 250 mg/kg

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

| | |
|---|---|
| Toxicity to fish | semi-static test LC50 - Brachydanio rerio (zebrafish) - ca. 75.6 mg/l - 96 h (OECD Test Guideline 203) |
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - Daphnia magna (Water flea) - 452 mg/l - 48 h (Regulation (EC) No. 440/2008, Annex, C.2) |
| Toxicity to algae | static test ErC50 - Desmodesmus subspicatus (green algae) - > 450 mg/l - 72 h (Regulation (EC) No. 440/2008, Annex, C.3) |
| Toxicity to bacteria | static test EC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209) |
| Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) | semi-static test EC50 - Daphnia magna (Water flea) - 16 mg/l - 21 d (OECD Test Guideline 211) |

12.2 Persistence and degradability

| | |
|------------------|--|
| Biodegradability | aerobic - Exposure time 28 d Result: 47.2 % - Not readily biodegradable. (ISO 10708) |
|------------------|--|

12.3 Bioaccumulative potential

| | |
|-----------------|---|
| Bioaccumulation | Cyprinus carpio (Carp) - 6 Weeks at 25 °C - 0.5 mg/l(1-chlorobutane) |
| | Bioconcentration factor (BCF): 7.6 - 21 (OECD Test Guideline 305C) |

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

No data available

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: 1127 Class: 3 Packing group: II
Proper shipping name: Chlorobutanes
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 1127 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: CHLOROBUTANES

IATA

UN number: 1127 Class: 3 Packing group: II
Proper shipping name: Chlorobutanes

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 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

1-chlorobutane 109-69-3

Pennsylvania Right To Know

1-chlorobutane 109-69-3

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 ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the 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.

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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