

SAFETY DATA SHEET

Version 6.7 Revision Date 10/27/2023 Print Date 07/13/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name: sec-ButylbenzeneProduct Number: B90408Brand: AldrichCAS-No.: 135-98-8

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 Acute toxicity, Oral (Category 4), H302 Short-term (acute) aquatic hazard (Category 1), H400 Long-term (chronic) aquatic hazard (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



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Signal Word	Warning
Hazard statement(s) H226 H302 H410	Flammable liquid and vapor. Harmful if swallowed. Very 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.
P270	Do not eat, drink or smoke when using this product.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
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	: 2-Phenylbutane
Formula	: C ₁₀ H ₁₄
Molecular weight	: 134.22 g/mol
CAS-No.	: 135-98-8
EC-No.	: 205-227-0

Component	Classification	Concentration
sec-Butylbenzene		
	Flam. Liq. 3; Acute Tox. 4; Aquatic Acute 1; Aquatic Chronic 1; H226, H302, H400, H410 M-Factor - Aquatic Acute: 1	<= 100 %

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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: 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 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 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

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

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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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

Change contaminated clothing. Preventive skin protection recommended. Wash hands 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.

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8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. 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

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact Material: Fluorinated rubber Minimum layer thickness: 0.7 mm Break through time: 480 min Material tested:Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Splash contact Material: Fluorinated rubber Minimum layer thickness: 0.7 mm Break through time: 480 min Material tested:Vitoject® (KCL 890 / Aldrich Z677698, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter type ABEK

The entrepeneur 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.

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SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

	•	, , ,	
a)	Appearance	Form: liquid, clear Color: colorless	
b)	Odor	No data available	
c)	Odor Threshold	No data available	
d)	рН	No data available	
e)	Melting point/freezing point	Melting point/range: 75.5 °C (167.9 °F) - lit.	
f)	Initial boiling point and boiling range	173 - 174 °C 343 - 345 °F - lit.	
g)	Flash point	52.0 °C (125.6 °F) - closed cup	
h)	Evaporation rate	No data available	
i)	Flammability (solid, gas)	No data available	
j)	Upper/lower flammability or explosive limits	Lower explosion limit: 0.8 %(V)	
k)	Vapor pressure	No data available	
I)	Vapor density	No data available	
m)	Density	0.863 g/mL at 25 °C (77 °F) - lit.	
	Relative density	No data available	
n)	Water solubility	No data available	
0)	Partition coefficient: n-octanol/water	No data available	
p)	Autoignition temperature	418.0 °C (784.4 °F)	
q)	Decomposition temperature	No data available	
r)	Viscosity	No data available	
s)	Explosive properties	No data available	
t)	Oxidizing properties	No data available	
Oth	Other safety information		

9.2 Other safety information No data available

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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: Strong oxidizing agents

- **10.4 Conditions to avoid** Heating.
- **10.5 Incompatible materials** various plastics
- **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 - 1,926 mg/kg Remarks: (RTECS) Inhalation: No data available LD50 Dermal - Rabbit - > 13,760 mg/kg Remarks: (RTECS) No data available

Skin corrosion/irritation

Skin - Rabbit Result: Mild eye irritant - 24 h Remarks: (RTECS)

Serious eye damage/eye irritation

Eyes - Rabbit Result: Mild eye irritation - 24 h Remarks: (RTECS)

Respiratory or skin sensitization No data available

Germ cell mutagenicity No data available

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

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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 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

RTECS: CY9100000

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

After absorption:

Headache Nausea narcosis

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - Daphnia magna (Water flea) - 0.6 mg/l - 48 h (OECD Test Guideline 202) Remarks: (in analogy to similar products)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 0.42 mg/l - 72 h (OECD Test Guideline 201) Remarks: (in analogy to similar products)
	static test NOEC - Pseudokirchneriella subcapitata (green algae) - 0.26 mg/l - 72 h (OECD Test Guideline 201) Remarks: (in analogy to similar products)

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12.2 Persistence and degradability No data available

- **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: 2709 Class: 3 Proper shipping name: Butyl benzenes	Packing group: III		
Reportable Quantity (RQ): Marine pollutant: yes Poison	Inhalation Hazard: No		
IMDG UN number: 2709 Class: 3 Proper shipping name: BUTYLBENZENE Marine pollutant : yes Marine pollutant : yes	Packing group: III S	EMS-No: F-E, S-D	
IATA UN number: 2709 Class: 3 Proper shipping name: Butylbenzenes	Packing group: III		

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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.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components		
sec-Butylbenzene	CAS-No. 135-98-8	Revision Date 1993-04-24
Pennsylvania Right To Know Components		Devision Data
sec-Butylbenzene	CAS-No. 135-98-8	Revision Date 1993-04-24
	122-98-8	1993-04-24

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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