

SAFETY DATA SHEET

Version 6.5
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Benzene-1,2-13C2

Product Number : 586218

Brand : Aldrich

Index-No. : 601-020-00-8

CAS-No. : 109432-78-2

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 2), H225

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Germ cell mutagenicity (Category 1B), H340

Carcinogenicity (Category 1A), H350

Specific target organ toxicity - repeated exposure (Category 1), Blood, H372

Aspiration hazard (Category 1), H304

Short-term (acute) aquatic hazard (Category 2), H401

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

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Pictogram



Signal word

Danger

Hazard statement(s)

H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H340	May cause genetic defects.
H350	May cause cancer.
H372	Causes damage to organs (Blood) through prolonged or repeated exposure.
H401	Toxic to aquatic life.
H412	Harmful to aquatic life with long lasting effects.

Precautionary statement(s)

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 dust/ fume/ gas/ mist/ vapors/ spray.
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/ protective clothing/ 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.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P331	Do NOT induce vomiting.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: 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.
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 : $^{13}\text{C}_2\text{C}_4\text{H}_6$
Molecular weight : 80.08 g/mol
CAS-No. : 109432-78-2
Index-No. : 601-020-00-8

Component	Classification	Concentration
Benzene-1,2-$^{13}\text{C}_2$		
	Flam. Liq. 2; Skin Irrit. 2; Eye Irrit. 2A; Muta. 1B; Carc. 1A; STOT RE 1; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 3; H225, H315, H319, H340, H350, H372, H304, H401, H412	<= 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: 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

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

Nature of decomposition products not known.

Combustible liquid.

Combustible.

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. 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

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.

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

Component	CAS-No.	Value	Control parameters	Basis
Benzene-1,2-13C2	109432-78-2	TWA	0.5 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Confirmed human carcinogen Danger of cutaneous absorption		
		STEL	2.5 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Leukemia Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Confirmed human carcinogen Danger of cutaneous absorption		
		TWA	0.1 ppm	USA. NIOSH Recommended Exposure Limits
		Potential Occupational Carcinogen		
		ST	1 ppm	USA. NIOSH Recommended Exposure Limits
		Potential Occupational Carcinogen		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Benzene-1,2-13C2	109432-78-2	S-Phenylmercapturic acid	25µg/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

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

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

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
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 5.5 °C (41.9 °F) - lit.
f) Initial boiling point and boiling range	80 °C 176 °F - lit.
g) Flash point	-11 °C (12 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	0.896 g/mL at 25 °C (77 °F) 0.896 g/cm ³ at 25 °C (77 °F)
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 | No data available |

9.2 Other safety information

No data available

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

No data available

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

Strong oxidizing agents

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 - > 2,000 mg/kg
(OECD Test Guideline 401)

Symptoms: Nausea

LC50 Inhalation - Rat - female - 4 h - 43.7 mg/l
(OECD Test Guideline 403)

LD50 Dermal - Rabbit - male and female - > 8,260 mg/kg
(OECD Test Guideline 402)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 4 h
(OECD Test Guideline 404)

Drying-out effect resulting in rough and chapped skin.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Eye irritation

Remarks: (ECHA)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

May cause genetic defects.

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Method: US-EPA

Result: positive

Test Type: In vitro mammalian cell gene mutation test

Metabolic activation: with and without metabolic activation

Method: US-EPA

Result: positive

Test Type: Mutagenicity (mammal cell test): micronucleus.

Species: Mouse

Cell type: Bone marrow

Application Route: inhalation (vapor)

Method: OECD Test Guideline 474

Result: positive

Carcinogenicity

May cause cancer. Positive evidence from human epidemiological studies.

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

Causes damage to organs through prolonged or repeated exposure. - Blood

Aspiration hazard

May be fatal if swallowed and enters airways.

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 120 d - NOAEL (No observed adverse effect level) - 100 mg/kg - LOAEL (Lowest observed adverse effect level) - 25 mg/kg

Remarks: Subchronic toxicity

Nausea, Dizziness, Headache, narcosis, Inhalation of high concentrations of benzene may have an initial stimulatory effect on the central nervous system characterized by exhilaration, nervous excitation and/or giddiness, depression, drowsiness, or fatigue. The victim may experience tightness in the chest, breathlessness, and loss of consciousness. Tremors, convulsions, and death due to respiratory paralysis or circulatory collapse can occur in a few minutes to several hours following severe exposures. Aspiration of small amounts of liquid immediately causes pulmonary edema and hemorrhage of pulmonary tissue. Direct skin contact may cause erythema. Repeated or prolonged skin contact may result in drying, scaling dermatitis, or development of secondary skin infections. The chief target organ is the hematopoietic system. Bleeding from the nose, gums, or mucous membranes and the development of purpuric spots, pancytopenia, leukopenia, thrombocytopenia, aplastic anemia, and leukemia may occur as the condition progresses. The bone marrow may appear normal, aplastic or hyperplastic, and may not correlate with peripheral blood-forming tissues. The onset of effects of prolonged benzene exposure may be delayed for many months or years after the actual exposure has ceased., Blood disorders

Systemic effects:

After absorption:

agitation
Headache
Dizziness
inebriation
Tiredness
CNS disorders
narcosis
respiratory arrest

Subacute toxicity

After a latency period:

Changes in the blood count
haemolysis

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	flow-through test LC50 - <i>Oncorhynchus mykiss</i> (rainbow trout) - 5.3 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic	static test EC50 - <i>Daphnia magna</i> (Water flea) - 10 mg/l - 48 h (OECD Test Guideline 202)

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invertebrates

Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 100 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test IC50 - - 13 mg/l - 24 h Remarks: (ECHA)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 96 % - Readily biodegradable. (OECD Test Guideline 301F)
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12.3 Bioaccumulative potential

Bioaccumulation	Leuciscus idus (Golden orfe) - 3 d - 0.05 mg/l(Benzene-1,2-13C2)
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Bioconcentration factor (BCF): 10

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 Other adverse effects

Endangers drinking-water supplies if allowed to enter soil or water.
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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 1114	Class: 3	Packing group: II
Proper shipping name: Benzene		
Reportable Quantity (RQ):		
Poison Inhalation Hazard: No		

IMDG

UN number: 1114	Class: 3	Packing group: II	EMS-No: F-E, S-D
Proper shipping name: BENZENE			

IATA

UN number: 1114	Class: 3	Packing group: II
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Proper shipping name: Benzene

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, Chronic Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

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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