

SAFETY DATA SHEET

Version 6.5
Revision Date 09/18/2021
Print Date 06/01/2022

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

Product name : Benzene-d₆

Product Number : 364940
Brand : Aldrich
CAS-No. : 1076-43-3

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

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

Synonyms : Hexadeutero benzene

Formula : C₆D₆

Molecular weight : 84.15 g/mol

CAS-No. : 1076-43-3

EC-No. : 214-061-8

Component	Classification	Concentration
(2H6)benzene		
	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

Move out of dangerous area. Consult a physician. Show this material safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

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

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion

Use explosion-proof equipment. **Advice on protection against fire and explosion**

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Handle and store under inert gas. hygroscopic

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

Component	CAS-No.	Value	Control parameters	Basis
(2H6)benzene	1076-43-3	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)
		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		
		PEL	1 ppm	OSHA Specifically Regulated Chemicals/Carcinogens
		OSHA specifically regulated carcinogen		
		STEL	5 ppm	OSHA Specifically Regulated Chemicals/Carcinogens
		OSHA specifically regulated carcinogen		
		TWA	10 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		CEIL	25 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Peak	50 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		PEL	1 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		STEL	5 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
(2H6)benzene	1076-43-3	S-Phenylmercaptopuric acid	25µg/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			
		t,t-Muconic acid	500µg/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			

8.2 Exposure controls**Appropriate engineering controls**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment**Eye/face protection**

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

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

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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: 6.8 °C (44.2 °F) - lit.
f) Initial boiling point and boiling range	79.1 °C 174.4 °F at 1,013 hPa - 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	Upper explosion limit: 8 %(V) Lower explosion limit: 1.3 %(V)
k) Vapor pressure	221 hPa at 37.7 °C (99.9 °F) 99.5 hPa at 20 °C(68 °F)
l) Vapor density	2.91 - (Air = 1.0)
m) Density	0.95 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	log Pow: 2.13 at 25 °C (77 °F)
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

Relative vapor density 2.91 - (Air = 1.0)

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Vapors may form explosive mixture with air.

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Acids, Bases, Halogens, Strong oxidizing agents, metal salts

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)

The value is given in analogy to the following substances: benzene

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

Dermal: No data available

No data available

Skin corrosion/irritation

Skin - Rabbit

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

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Eye irritation

Remarks: (ECHA)

The value is given in analogy to the following substances: benzene

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

The value is given in analogy to the following substances: benzene

Carcinogenicity

May cause cancer. Positive evidence from human epidemiological studies.

IARC: 1 - Group 1: Carcinogenic to humans ((2H6)benzene)

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

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.

Blood - Irregularities - Based on Human Evidence

Blood - 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 algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> - 100 mg/l - 72 h

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(OECD Test Guideline 201)

12.2 Persistence and degradability

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

12.3 Bioaccumulative potential

Bioaccumulation Leuciscus idus (Golden orfe) - 3 d
- 0.05 mg/l((2H6)benzene)

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

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Harmful to aquatic life with long lasting 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

Contact a licensed professional waste disposal service to dispose of this material. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

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

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: BENZENESOLUTION

IATA

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SECTION 15: Regulatory information

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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

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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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Version: 6.5

Revision Date: 09/18/2021

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