

SAFETY DATA SHEET

Version 8.11
Revision Date 09/06/2024
Print Date 09/07/2024

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

1.1 Product identifiers

Product name : Benzene-d
Product Number : 175722
Brand : Aldrich
Index-No. : 601-020-00-8
CAS-No. : 1120-89-4, 119516-83-5

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

Identified uses : Laboratory chemicals, Synthesis of substances
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
Eye irritation (Category 2A), H319

Aldrich - 175722

Page 1 of 14

The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

Millipore
Sigma

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 Statements

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 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.
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	: C ₆ DH ₅
Molecular weight	: 79.12 g/mol
CAS-No.	: 1120-89-4
EC-No.	: 214-321-0
Index-No.	: 601-020-00-8

Component	Classification	Concentration
Benzene-d1		
	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**

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.

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

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-d1	1120-89-4	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
Benzene-d1	1120-89-4	S-Phenylmercaptoacetic 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

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: 10 min

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

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter A-(P3)

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
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	0.885 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	none

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

Exothermic reaction with:

halogens

Halogenated hydrocarbon

in the presence of:

Light metals

Risk of explosion with:

halogen-halogen compounds

Nitric acid

Boranes

Ozone

peroxy compounds
perchlorates
permanganic acid
perchloryl fluoride
Strong oxidizing agents
Chlorine
fluorides
uranium hexafluoride
Oxygen
liquid
Risk of ignition or formation of inflammable gases or vapours with:
chromium(VI) oxide
Fluorine
nitryl compounds
Oxygen
oxyhalogenic compounds
Violent reactions possible with:
mineral acids
sulfur

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

LD50 Oral - Rat - male - > 2,000 mg/kg
(OECD Test Guideline 401)

Symptoms: Nausea

LC50 Inhalation - Rat - female - 4 h - 43.7 mg/l - vapor

(OECD Test Guideline 403)

Symptoms: Possible damages:, mucosal irritations

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

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 4 h

(OECD Test Guideline 404)

Remarks: 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: 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: 1 - Group 1: Carcinogenic to humans (Benzene-d1)

NTP: Known - Known to be human carcinogen (Benzene-d1)

OSHA: OSHA specifically regulated carcinogen (Benzene-d1)

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

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Aspiration hazard

Aspiration may cause pulmonary edema and pneumonitis.

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

Aldrich - 175722

Page 10 of 14

Remarks: Subchronic toxicity

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 invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - 10 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - 100 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - <i>Pimephales promelas</i> (fathead minnow) - 0.8 mg/l - 32 d Remarks: (ECHA)
Toxicity to daphnia and other aquatic	semi-static test NOEC - <i>Ceriodaphnia dubia</i> (water flea) - 3 mg/l - 7 d

invertebrates(Chronic (US-EPA) toxicity)

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(Benzene-d1)

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 Endocrine disrupting properties

No data available

12.7 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.

SECTION 14: Transport information

DOT (US)

UN number: 1114 Class: 3 Packing group: II
Proper shipping name: Benzene
Reportable Quantity (RQ): 10 lbs
Reportable Quantity (RQ): 10 lbs
Poison Inhalation Hazard: No

IMDG

Aldrich - 175722

Page 12 of 14

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**MILLIPORE
SIGMA**

UN number: 1114
E, S-D
Proper shipping name: BENZENE

Class: 3

Packing group: II EMS-No: F-

IATA
UN number: 1114 Class: 3
Proper shipping name: Benzene

Packing group: II

SECTION 15: Regulatory information

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Benzene-d1	1120-89-4	10	10
Benzene-d1	1120-89-4	10	10 (D018)

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 311/312

Hazards

- : Fire Hazard
- Acute Health Hazard
- Chronic Health Hazard

SARA 313

- : The following components are subject to reporting levels established by SARA Title III, Section 313:

Benzene-d1 1120-89-4 >= 90 - <= 100 %

US State Regulations

Massachusetts Right To Know

Benzene-d1 1120-89-4

Pennsylvania Right To Know

Benzene-d1 1120-89-4

Maine Chemicals of High Concern

Benzene-d1 1120-89-4

Vermont Chemicals of High Concern

Benzene-d1 1120-89-4

Washington Chemicals of High Concern

Benzene-d1 1120-89-4

California Prop. 65

WARNING: This product can expose you to chemicals including Benzene-d1, which is/are known to the State of California to cause cancer and birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov.

The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on 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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

Details in analogy to the undeuterated compound.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 8.11

Revision Date: 09/06/2024

Print Date: 09/07/2024