

SAFETY DATA SHEET

Version 8.8
Revision Date 26.08.2021
Print Date 26.02.2023**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**Product name : Benzene-D6 deuteration degree min. 99.95%
for NMR spectroscopy MagniSolv™Product Number : 1.01766
Catalogue No. : 101766
Brand : Millipore
CAS-No. : 1076-43-3**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Reagent for analysis

1.3 Details of the supplier of the safety data sheetCompany : SIGMA-ALDRICH CANADA LTD.
2149 WINSTON PARK DRIVE
OAKVILLE ON L6H 6J8
CANADATelephone : +1 905 829-9500
Fax : +1 905 829-9292**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 Hazardous Products Regulations (HPR)
(SOR/2015-17)**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, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.
P240	Ground and bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use non-sparking tools.
P243	Take action to prevent static discharges.
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.
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 + P364	Take off contaminated clothing and wash it 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 : C6D6
Molecular weight : 84.16 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 %
* Weight %		

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. Chemisorb®). 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.

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

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
(2H6)benzene	1076-43-3	STEL	2.5 ppm 8 mg/m ³	Canada. Alberta, Occupational Health and Safety Code (table 2: OEL)
Remarks	Confirmed Human Carcinogen (means that the agent is carcinogenic to humans) Substance may be readily absorbed through intact skin			
		TWA	0.5 ppm 1.6 mg/m ³	Canada. Alberta, Occupational Health and Safety Code (table 2: OEL)
	Confirmed Human Carcinogen (means that the agent is carcinogenic to humans) Substance may be readily absorbed through intact skin			
		TWA	0.5 ppm	Canada. British Columbia OEL
	IARC '1' applies to substances categorized as carcinogenic to humans, and used when there is sufficient evidence of carcinogenicity in humans. ACGIH 'A1' applies to those substances confirmed as human carcinogens based on the weight of evidence from epidemiological studies Contributes significantly to the overall exposure by the skin route.			
		STEL	2.5 ppm	Canada. British Columbia OEL
	IARC '1' applies to substances categorized as carcinogenic to humans, and used when there is sufficient evidence of carcinogenicity in humans. ACGIH 'A1' applies to those substances confirmed as human carcinogens based on the weight of evidence from epidemiological studies Contributes significantly to the overall exposure by the skin route.			

		TWA	0.5 ppm	Ontario Table of Occupational Exposure Limits made under the Occupational Health and Safety Act.
	Skin			
		STEL	2.5 ppm	Ontario Table of Occupational Exposure Limits made under the Occupational Health and Safety Act.
	Skin			
		TWAEV	1 ppm 3 mg/m ³	Québec. Regulation respecting occupational health and safety, Schedule 1, Part 1: Permissible exposure values for airborne contaminants
	Carcinogenic effect detected in humans			
		STEV	5 ppm 15.5 mg/m ³	Québec. Regulation respecting occupational health and safety, Schedule 1, Part 1: Permissible exposure values for airborne contaminants
	Carcinogenic effect detected in humans			
		TWA	0.5 ppm	USA. ACGIH Threshold Limit Values (TLV)
		STEL	2.5 ppm	USA. ACGIH Threshold Limit Values (TLV)

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 EN374 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 EN374 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

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 | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | No data available |
| f) Initial boiling point and boiling range | 79.1 °C 174.4 °F at 1,013 hPa |
| 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 | 99.5 hPa at 20 °C (68 °F) |
| l) Vapor density | 2.91 - (Air = 1.0) |
| m) Density | 0.95 g/cm ³ at 20 °C (68 °F) |
| Relative density | No data available |
| n) Water solubility | No data available |

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- o) Partition coefficient: No data available
n-octanol/water
- p) Autoignition No data available
temperature
- q) Decomposition No data available
temperature
- r) Viscosity No data available
- s) Explosive properties No data available
- t) Oxidizing properties none

9.2 Other safety information

Relative vapor density 2.91 - (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

Exothermic reaction with:

halogens

uranium hexafluoride

Halogenated hydrocarbon

in the presence of:

Light metals

Risk of explosion with:

halogen-halogen compounds

Nitric acid

Ozone

peroxi compounds

perchlorates

permanganic acid

perchloryl fluoride

Strong oxidizing agents

Chlorine

fluorides

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

rubber, 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 - 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

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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.

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

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish flow-through test LC50 - *Oncorhynchus mykiss* (rainbow trout) - 5.3 mg/l - 96 h
(OECD Test Guideline 203)

Toxicity to algae static test ErC50 - *Pseudokirchneriella subcapitata* - 100 mg/l - 72 h
(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

Biological 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

TDG

UN number: 1114 Class: 3 Packing group: II
Proper shipping name: BENZENE
Labels: 3
ERG Code: 130
Marine pollutant: 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
Proper shipping name: Benzene

SECTION 15: Regulatory information

This product has been classified in accordance with the hazard criteria of the Hazardous Products Regulations (HPR) and the SDS contains all the information required by the HPR.

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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Details in analogy to the undeuterated compound.

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Version: 8.8

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