

Chemical Safety Data Sheet MSDS / SDS

Benzene-D6

Revision Date:2023-12-30 Revision Number:1

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

Product identifier

Product name : Benzene-D6
CBnumber : CB3685998
CAS : 1076-43-3
EINECS Number : 214-061-8
Synonyms : benzene-d6,hexadeuterobenzene

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P201 Obtain special instructions before use.
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P303+P361+P353 IF ON SKIN (or hair): Remove/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. Continuerinsing.
P308+P313 IF exposed or concerned: Get medical advice/attention.
P370+P378 In case of fire: Use ... for extinction.
P403+P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.

Hazard statements

H225 Highly Flammable liquid and vapour
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
H370 Causes damage to organs
H372 Causes damage to organs through prolonged or repeated exposure
H412 Harmful to aquatic life with long lasting effects

SECTION 3: Composition/information on ingredients

Substance

Product name	: Benzene-D6
Synonyms	: benzene-d6,hexadeuterobenzene
CAS	: 1076-43-3
EC number	: 214-061-8
MF	: C6D6
MW	: 84.15

SECTION 4: First aid measures

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.

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

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.

Special hazards arising from the substance or mixture

Carbon oxides Not combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors. Forms explosive mixtures with air at ambient temperatures. Ambient fire may liberate hazardous vapours.

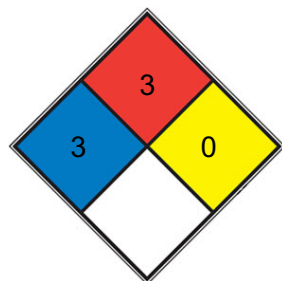
Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

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

NFPA 704



<input checked="" type="checkbox"/>	HEALTH	3	Short exposure could cause serious temporary or moderate residual injury (e.g. liquid hydrogen , sulfuric acid , calcium hypochlorite , hexafluorosilicic acid)
<input checked="" type="checkbox"/>	FIRE	3	Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions. Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, acetone)
<input checked="" type="checkbox"/>	REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N₂)
<input type="checkbox"/>	SPEC.		
<input type="checkbox"/>	HAZ.		

SECTION 6: Accidental release measures

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.

Environmental precautions

Do not let product enter drains. Risk of explosion.

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.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

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.

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.

Handle and store under inert gas. hygroscopic

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

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

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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	colorless liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 6,8 °C - lit.
Initial boiling point and boiling range	79,1 °C at 1.013 hPa - lit.
Flash point	-11 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive	Upper explosion limit: 8 %(V) Lower explosion limit: 1,3 %(V)

limits

Vapour pressure	99,5 hPa at 20 °C
Vapour density	2,91 - (Air = 1.0)
Relative density	0.950
Water solubility	Miscible with most organic solvents.
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

Relative vapor density

2,91 - (Air = 1.0)

SECTION 10: Stability and reactivity

Reactivity

Vapors may form explosive mixture with air.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

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

Conditions to avoid

Warming.

Incompatible materials

rubber, various plastics

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

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

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

(OECD Test Guideline 406)

Germ cell mutagenicity

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

No data available

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.

Toxicity

LD50 orally in Rabbit: 930 mg/kg LD50 dermal Rabbit > 8260 mg/kg

SECTION 12: Ecological information

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)

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 96 % - Readily biodegradable. (OECD Test Guideline 301F)

Bioaccumulative potential

Bioaccumulation *Leuciscus idus* (Golden orfe) - 3 d

- 0,05 mg/l((2H6)benzene)

Bioconcentration factor (BCF): 10

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

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

Waste treatment methods

Product

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

UN number

ADR/RID: 1114 IMDG: 1114

UN proper shipping name

ADR/RID: BENZENE IMDG: BENZENE IATA: Benzene

Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

Packaging group

ADR/RID: II IMDG: II IATA: II

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

EC Inventory:Listed.

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Disclaimer:

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