

Chemical Safety Data Sheet MSDS / SDS

Benzyl mercaptan

Revision Date:2025-02-01 Revision Number:1

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

Product identifier

Product name : Benzyl mercaptan
CBnumber : CB0680361
CAS : 100-53-8
EINECS Number : 202-862-5
Synonyms : phenylmethanethiol,benzyl mercaptan

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 : 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P501 Dispose of contents/container to....
P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P391 Collect spillage. Hazardous to the aquatic environment
P370+P378 In case of fire: Use ... for extinction.
P310 Immediately call a POISON CENTER or doctor/physician.
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.
P284 Wear respiratory protection.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P273 Avoid release to the environment.

P271 Use only outdoors or in a well-ventilated area.
P270 Do not eat, drink or smoke when using this product.
P264 Wash skin thoroughly after handling.
P264 Wash hands thoroughly after handling.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

Hazard statements

H302 Harmful if swallowed
H315 Causes skin irritation
H319 Causes serious eye irritation
H330 Fatal if inhaled
H400 Very toxic to aquatic life
H410 Very toxic to aquatic life with long lasting effects
H227 Combustible liquid

SECTION 3: Composition/information on ingredients

Substance

Product name	: Benzyl mercaptan
Synonyms	: phenylmethanethiol, benzyl mercaptan
CAS	: 100-53-8
EC number	: 202-862-5
MF	: C ₇ H ₈ S
MW	: 124.2

SECTION 4: First aid measures

Description of first aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

Water Foam Carbon dioxide (CO₂) 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 Sulfur oxides Combustible.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

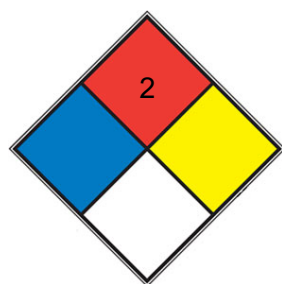
Advice for firefighters

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. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

NFPA 704



■ HEALTH

Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely

■ FIRE 2 divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

■ REACT

SPEC.

□ 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.

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

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

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 Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,40 mm Break through time: 60 min

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

Full contact

Material: butyl-rubber

Minimum layer thickness: 0,70 mm Break through time: 480 min Material tested: Butoject? (KCL 898)

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

protective clothing

Respiratory protection

Recommended Filter type: Filter type B

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.

Skin protection

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 Splash contact Material: Nitrile rubber

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Control of environmental exposure

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SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	liquid
Odour	stinging
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point: -29,2 °C
Initial boiling point and boiling range	194 - 195 °C - lit.
Flash point	158 °F
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Lower explosion limit: 1 %(V)
Vapour pressure	0,5 hPa at 20 °C
Vapour density	>4 (vs air)
Relative density	No data available
Water solubility	at 20 °C practically insoluble
Partition coefficient: n-octanol/water	log Pow: 2,48 at 25 °C - Bioaccumulation is not expected.
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

No data available

SECTION 10: Stability and reactivity

Reactivity

Forms explosive mixtures with air on intense heating.

Chemical stability

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

Possibility of hazardous reactions

Violent reactions possible with: Strong oxidizing agents

Strong acids

Conditions to avoid

Strong heating.

Incompatible materials

No data available

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 493 mg/kg Remarks: (RTECS)absorption

LC50 Inhalation - Mouse - 4 h - 0,9 mg/l Remarks: (External MSDS)

Skin corrosion/irritation

Skin - Rabbit

Result: slight irritation Remarks: (External MSDS)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: slight irritation Remarks: (External MSDS)

Respiratory or skin sensitization

Remarks:

(External MSDS)

Germ cell mutagenicity

Test Type: Ames test Result: negative Remarks: (Lit.)

Carcinogenicity

No data available

Reproductive toxicity

Specific target organ toxicity - single exposure Specific target organ toxicity - repeated exposure Aspiration hazard

SECTION 12: Ecological information

Toxicity

Toxicity to daphnia and other aquatic invertebrates

EC50 - Daphnia magna (Water flea) - 0,15 mg/l - 48 h (OECD Test Guideline 202)

Persistence and degradability

Biodegradability Result: 40,7 % - Not readily biodegradable.

Remarks: (External MSDS)

Bioaccumulative potential

Mobility in soil

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

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: 2810 IMDG: 2810 IATA: 2810

UN proper shipping name

ADR/RID: TOXIC LIQUID, ORGANIC, N.O.S. (benzyl mercaptan) IMDG: TOXIC LIQUID, ORGANIC, N.O.S. (benzyl mercaptan) IATA: Toxic liquid, organic, n.o.s. (benzyl mercaptan)

Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

Packaging group

ADR/RID: II IMDG: II IATA: II

Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes 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: 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.

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

Philippines Inventory of Chemicals and Chemical Substances (PICCS): Listed. website: <https://emb.gov.ph/>

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

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

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

Vietnam National Chemical Inventory: Listed. website: <https://chemicaldata.gov.vn/>

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:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.