Chemical Safety Data Sheet MSDS / SDS

Benzotrichloride

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

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

Product identifier

Product name : Benzotrichloride
CBnumber : CB6339243
CAS : 98-07-7
EINECS Number : 202-634-5

Synonyms : Benzotrichloride,(trichloromethyl)benzene

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

P405 Store locked up.

P320 Specific treatment is urgent (see ... on this label).

P311 Call a POISON CENTER or doctor/physician.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P201 Obtain special instructions before use.

Hazard statements

H350 May cause cancer

H335 May cause respiratory irritation

H331 Toxic if inhaled

H330 Fatal if inhaled

H318 Causes serious eye damage

H315 Causes skin irritation

H314 Causes severe skin burns and eye damage

H302 Harmful if swallowed

Disposal

WARNING.Cancer - https://oehha.ca.gov/proposition-65/chemicals/benzotrichloride

SECTION 3: Composition/information on ingredients

Substance

Product name : Benzotrichloride

Synonyms : Benzotrichloride,(trichloromethyl)benzene

CAS : 98-07-7
EC number : 202-634-5
MF : C7H5Cl3
MW : 195.47

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. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. 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 Hydrogen chloride gas Combustible.

Vapors are heavier than air and may spread along floors. Risk of dust explosion.

Forms explosive mixtures with air on intense heating.

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

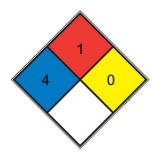
Advice for firefighters

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

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 4

FIRE

Very short exposure could cause death or major residual injury (e.g. hydrogen cyanide, phosgene, methyl isocyanate, hydrofluoric acid)

Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion

1 can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. mineral oil, ammonia)

 \blacksquare REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N_2)

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. 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 liquidabsorbent material (e.g.

Chemizorb?). 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.

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

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

Moisture sensitive.

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). Tightly fitting safety goggles

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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

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: Nitrile rubber

Minimum layer thickness: 0,2 mm Break through time: 49 min

Material tested:Dermatril? P (KCL 743 / Aldrich Z677388, 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

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.

Recommended Filter type: Filter type ABEK

The entrepeneur 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.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	light yellow clear, liquid
Odour	pungent
Odour Threshold	No data available
рН	No data available
Melting point/freezing point	Melting point/range: -7,57 °C - lit.
Initial boiling point and boiling range	219 - 223 °C at 1.013 hPa - lit. 90 - 91 °C at 20 hPa - lit.
Flash point	109 °C - closed cup
Evaporation rate	No data available

	Upper explosion limit: 6,5 %(V) Lower explosion limit: 2,1 %(V)
Upper/lower flammability or explosive	Speci supression minit. 6,6 %(v) Edwar explosion minit. 2,1 %(v)
limits	
Vapour pressure	3 hPa at 55 °C 0,3 hPa at 20 °C
Vapour density	6,75 - (Air = 1.0)
Relative density	1,38 g/cm3 at 25 °C - lit. No data available
Water solubility	alcohol: soluble
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	211 °C at 1.013 hPa
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: 2,4 mPa.s at 20 °C
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

Relative vapor density

6,75 - (Air = 1.0)

SECTION 10: Stability and reactivity

Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

Chemical stability

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

Possibility of hazardous reactions

No data available

Conditions to avoid

Strong heating.

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - 1.590 mg/kg

(OECD Test Guideline 401)

Acute toxicity estimate Inhalation - 4 h - 5 mg/l (Expert judgment)

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

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

Symptoms: Inhalation may lead to the formation of oedemas in the respiratory tract., mucosal irritations, Cough, Shortness of breath, Possible

damages:, damage of respiratory tract

LD50 Dermal - Rabbit - 4.000 mg/kg Remarks: Behavioral:Excitement.

Liver:Other changes.

Prolonged skin contact may cause skin irritation and/or dermatitis. (RTECS)

Skin corrosion/irritation

Causes skin irritation. Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Serious eye damage/eye irritation

Causes serious eye damage. Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium Metabolic activation: with and without metabolic activation Method: OECD Test Guideline

471

Result: positive

Remarks: (National Toxicology Program)

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause respiratory irritation. - Skin, Lungs

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

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Toxicity

LD50 orally in rats: 6.0 g/kg (Smyth)

SECTION 12: Ecological information

Toxicity

Toxicity to fish

LC50 - Pimephales promelas (fathead minnow) - 6 mg/l - 96 h Remarks: (External MSDS)

Toxicity to daphnia and other aquatic invertebrates

EC50 - Daphnia magna (Water flea) - > 100 mg/l - 48 h Remarks: (Lit.)

Toxicity to bacteria

microtox test EC50 - Photobacterium phosphoreum - 17,83 mg/l - 30 min

Remarks: (IUCLID)

Persistence and degradability

Biodegradability aerobic - Exposure time 7 d

Result: 97 % - Readily biodegradable. (OECD Test Guideline 301E)

Bioaccumulative potential

No data available

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

Biological effects:

Forms corrosive mixtures with water even if diluted. Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Waste treatment methods

Incompatibilities

Benzotrichloride decomposes on heating, on contact with acids and/or water, producing toxic and corrosive hydrogen chloride and benzoic acid. Reacts violently with strong oxidizers, iron and other metals, alkali and earth alkali metals; bases and organic substances.

Product

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

Waste Disposal

Incineration with flammable solvent added in incinerator with afterburner and alkaline scrubber.

SECTION 14: Transport information

UN number

ADR/RID: 2226 IMDG: 2226 IATA: 2226

UN proper shipping name

ADR/RID: BENZOTRICHLORIDE IMDG: BENZOTRICHLORIDE

IATA: Benzotrichloride

Transport hazard class(es) 14.3

ADR/RID: 8 IMDG: 8 IATA: 8

Packaging group 14.4

ADR/RID: II IMDG: II IATA: II

Environmental hazards 14.5

ADR/RID: no IMDG Marine pollutant: no

IATA: no

Special precautions for user 14.6

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

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

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

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):Listed. website: http://ncis.nier.go.kr

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

EC Inventory:Listed.

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

SECTION 16: Other information

Abbreviations and acronyms

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

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association
IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

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

STEL: Short term exposure limit TWA: Time Weighted Average

References

- [1] CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- [2] ChemlDplus, 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/

Other Information

Combustible vapour/air mixtures difficult to ignite, may be developed under certain conditions. The occupational exposure limit value should not be exceeded during any part of the working exposure. Depending on the degree of exposure, periodic medical examination is suggested. Refer for medical attention if breathing difficulties and/or fever develop.

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.