ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

4-Chlorobenzotrifluoride

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

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

Product identifier

Product name	: 4-Chlorobenzotrifluoride
CBnumber	: CB9854750
CAS	: 98-56-6
EINECS Number	: 202-681-1
Synonyms	: 4-Chlorobenzotrifluoride,PCBTF

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 Warning

Precautionary statements

P501 Dispose of contents/container to.....

P405 Store locked up.

P403+P235 Store in a well-ventilated place. Keep cool.

P391 Collect spillage. Hazardous to the aquatic environment

P333+P313 IF SKIN irritation or rash occurs: Get medical advice/attention.

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

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.

P273 Avoid release to the environment.

P264 Wash skin thouroughly after handling.

P264 Wash hands thoroughly after handling.

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

P240 Ground/bond container and receiving equipment.

P233 Keep container tightly closed.

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

Hazard statements

H411 Toxic to aquatic life with long lasting effects

H335 May cause respiratory irritation

H319 Causes serious eye irritation

H317 May cause an allergic skin reaction

H315 Causes skin irritation

H226 Flammable liquid and vapour

SECTION 3: Composition/information on ingredients

Substance

Product name	: 4-Chlorobenzotrifluoride
Synonyms	: 4-Chlorobenzotrifluoride,PCBTF
CAS	: 98-56-6
EC number	: 202-681-1
MF	: C7H4ClF3
MW	: 180.55

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

Dry powder Dry sand

Unsuitable extinguishing media

Do NOT use water jet.

Special hazards arising from the substance or mixture

Carbon oxides, Hydrogen chloride gas, Hydrogen fluoride

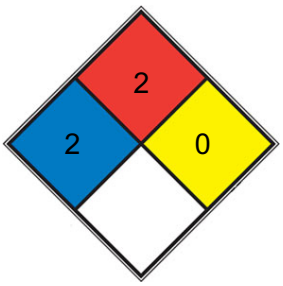
Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

Use water spray to cool unopened containers.

NFPA 704



■	HEALTH	2	Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. diethyl ether, ammonium phosphate, iodine)
■	FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely 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	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,N2)
□	SPEC. HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Store in cool place.

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

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

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.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	colorless clear, viscous liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: -36 °C - lit.
Initial boiling point and boiling range	136 - 138 °C - lit.
Flash point	43 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	0,000 hPa at 25 °C - OECD Test Guideline 104
Vapour density	No data available
Relative density	1,353 g/cm3 at 25 °C - lit.
Water solubility	0,0338 g/l at 20 °C - slightly soluble
Partition coefficient: n-octanol/water	log Pow: 3,7 at 25 °C
Autoignition temperature	log Pow: 3,7 at 25 °C
Decomposition temperature	No data available
Viscosity	0,76 mm2/s at 20 °C - 0,58 mm2/s at 40 °C -
Explosive properties	Not explosive
Oxidizing properties	No data available

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

Heat, flames and sparks.

Incompatible materials

Strong bases, Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen chloride gas, Hydrogen fluoride

Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 13.000 mg/kg

LD50 Oral - Rat - 5.546 mg/kg

LC50 Inhalation - Rat - 4 h - > 32,03 mg/l LD50 Dermal - Rabbit - > 3.300 mg/kg

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

Respiratory or skin sensitization

in vivo assay - Mouse

May cause sensitization by skin contact. (OECD Test Guideline 429)

Germ cell mutagenicity

Ames test

Salmonella typhimurium

Result: Not mutagenic in Ames Test. Chromosome aberration test in vitro Chinese hamster ovary cells

Result: negative

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

RTECS: XS9145000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

Toxicity

Toxicity to fish

semi-static test LC50 - Danio rerio (zebra fish) - 3 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates

EC50 - Daphnia magna (Water flea) - 2 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae

NOEC - Pseudokirchneriella subcapitata (green algae) - 0,41 mg/l - 72 h

(OECD Test Guideline 201)

Persistence and degradability

Biodegradability Result: - According to the results of tests of biodegradability this product is not readily biodegradable.

(OECD Test Guideline 301D)

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.

Toxics Screening Level

The current initial threshold screening level (ITSL) for p-chlorobenzotrifluoride is 70 µg/m3 based on an annual averaging time.

Other adverse effects

Toxic to aquatic life with long lasting effects. No data available

---

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Incompatibilities

Vapors may form explosive mixture with air. Violent reaction with strong oxidizers, such as permanganates and dichromates, chlorates, nitrates, peroxides, perchlorates, chlorine, bromine, fluorine, etc.; contact may cause fires or explosions. Keep away from alkaline materials, strong bases, strong acids, oxoacids, epoxides.

Waste Disposal

In accordance with 40CFR165 recommendations for the disposal of pesticides and pesticide containers. Must be disposed properly by following package label directions or by contacting your local or federal environmental control agency, or by contacting your regional EPA office.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 2234 IMDG: 2234 IATA: 2234

UN proper shipping name

ADR/RID: CHLOROBENZOTRIFLUORIDES IMDG: CHLOROBENZOTRIFLUORIDES

IATA: Chlorobenzotrifluorides

14.3	Transport hazard class(es) ADR/RID: 3 IMDG: 3	IATA: 3
14.4	Packaging group ADR/RID: III IMDG: III	IATA: III
14.5	Environmental hazards ADR/RID: no IMDG Marine pollutant: no	IATA: no
14.6	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

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

EC Inventory:Listed.

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

Korea Existing Chemicals List (KECL):Listed. website: http://ncis.nier.go.kr

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

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

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

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

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】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.