Chemical Safety Data Sheet MSDS / SDS

1-Bromo-4-(trifluoromethoxy)benzene

Revision Date: 2024-12-07 Revision Number: 1

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

Product identifier

Product name : 1-Bromo-4-(trifluoromethoxy)benzene

CBnumber : CB1413764

CAS : 407-14-7

EINECS Number : 206-979-2

Synonyms : 1-bromo-4-(trifluoromethoxy)benzene,4-(trifluoromethoxy)bromobenzene

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

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

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

P264 Wash hands thoroughly after handling.

P264 Wash skin thouroughly after handling.

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

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

Continuerinsing.

P342+P311 IF experiencing respiratory symptoms: call a POISON CENTER or doctor/physician.

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

P405 Store locked up.

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

Hazard statements

H227 Combustible liquid

H302 Harmful if swallowed

H303 May be harmfulif swallowed

H315 Causes skin irritation

H319 Causes serious eye irritation

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled

H335 May cause respiratory irritation

SECTION 3: Composition/information on ingredients

Substance

Product name : 1-Bromo-4-(trifluoromethoxy)benzene

Synonyms : 1-bromo-4-(trifluoromethoxy)benzene,4-(trifluoromethoxy)bromobenzene

CAS : 407-14-7
EC number : 206-979-2
MF : C7H4BrF3O
MW : 241.01

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

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

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

Small (incipient) fires must be extinguished with alcohol resistant foam, dry chemical powder or carbon dioxide. Large amounts of water are ineffective. Cool containers with large amounts of water.

Special hazards arising from the substance or mixture

Carbon oxides Hydrogen bromide gas Hydrogen fluoride

Advice for firefighters

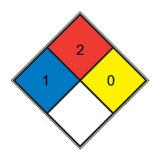
Wear self-contained breathing apparatus for firefighting if necessary.

Further information

Use water spray to cool unopened containers.

NFPA 704

FIRE



■ HEALTH 1 Exposure would cause irritation with only minor residual injury (e.g. acetone, sodium bromate, potassium chloride)

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, <u>sulfur</u>)

■ 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. Evacuate personnel to safe areas. 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 an electrically protected vacuum cleaner or by wet- brushing and place in container for disposal

according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Advice on safe handling

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

Advice on protection against fire and explosion

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

Hygiene measures

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

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Store in cool place. 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.

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

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, 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, liquid
Odour	No data available
Odour Threshold	No data available
рН	No data available
Melting point/freezing point	No data available
Initial boiling point and boiling range	80 °C at 67 hPa - lit.
Flash point	68 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive	No data available
limits	
Vapour pressure	20 hPa (55 °C)
Vapour density	No data available
Relative density	1.64
Water solubility	11.7mg/l
Partition coefficient: n-octanol/water	log Pow. 3,928
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

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 oxidizing agents

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - 500 mg/kg (Calculation method)

LD50 Oral - Rat - > 2.500 mg/kg

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Remarks: (External MSDS)

Skin corrosion/irritation

Skin - Rabbit Result: Irritations

Remarks: (External MSDS)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation Remarks: (External MSDS)

Respiratory or skin sensitization

Germ cell mutagenicity

Test Type: Ames test Result: negative

Remarks: (External MSDS)

Carcinogenicity

No data available

Reproductive toxicity

Specific target organ toxicity - single exposure

Specific target organ toxicity - repeated exposure Aspiration hazard

Toxicity

LD50 orally in Rabbit: > 2500 mg/kg

SECTION 12: Ecological information

Toxicity

Toxicity to fish

LC0 - Danio rerio (zebra fish) - > 11,7 mg/l - 96 h

Remarks: (above the solubility limit in the test medium) (External MSDS)

Toxicity to bacteria

Persistence and degradability

Biodegradability Result: 1 % - Not readily biodegradable.

(OECD Test Guideline 301D)

Bioaccumulative potential

Mobility in soil

Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

Other adverse effects

Toxic to aquatic life.

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Waste treatment methods

Product

This combustible material may be burned in a chemical incinerator equipped with an

afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 3082 IMDG: 3082 IATA: 3082

UN proper shipping name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (1-bromo-4-

(trifluoromethoxy)benzene)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (1-bromo-4-

(trifluoromethoxy)benzene)

IATA: Environmentally hazardous substance, liquid, n.o.s. (1-bromo-4- (trifluoromethoxy)benzene)

Transport hazard class(es)

ADR/RID: 9 IMDG: 9 IATA: 9

Packaging group

ADR/RID: III IMDG: III IATA: III

Environmental hazards

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

Special precautions for user

Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

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

EC Inventory:Listed.

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

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

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: https://www.mee.gov.cn/

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

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: https://www.epa.govt.nz/

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

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: https://www.epa.gov/

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

- [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
- [1] CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- [2] ChemlDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
- 【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.