

## Chemical Safety Data Sheet MSDS / SDS

## 4-Bromomethyl-2-cyanobiphenyl

Revision Date:2025-06-28 Revision Number:1

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

## Product identifier

Product name : 4-Bromomethyl-2-cyanobiphenyl  
CBnumber : CB2685168  
CAS : 114772-54-2  
EINECS Number : 425-280-5  
Synonyms : br-otbn,4'-(bromomethyl)-[1,1'-biphenyl]-2-carbonitrile

## 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

Warning

## Precautionary statements

P273 Avoid release to the environment.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.  
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.  
P405 Store locked up.  
P501 Dispose of contents/container to.....  
P270 Do not eat, drink or smoke when using this product.  
P264 Wash skin thoroughly after handling.

P264 Wash hands thoroughly after handling.

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

P202 Do not handle until all safety precautions have been read and understood.

P201 Obtain special instructions before use.

#### **Hazard statements**

H302 Harmful if swallowed

H312 Harmful in contact with skin

H315 Causes skin irritation

H317 May cause an allergic skin reaction

H319 Causes serious eye irritation

H331 Toxic if inhaled

H335 May cause respiratory irritation

H341 Suspected of causing genetic defects

H410 Very toxic to aquatic life with long lasting effects

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: 4-Bromomethyl-2-cyanobiphenyl
Synonyms	: br-otbn,4'-(bromomethyl)-[1,1'-biphenyl]-2-carbonitrile
CAS	: 114772-54-2
EC number	: 425-280-5
MF	: C14H10BrN
MW	: 272.14

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## 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**

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

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Hydrogen bromide gas

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### Further information

No data available

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

☒ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

☐ SPEC.

☐ HAZ.

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## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

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

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

## Reference to other sections

For disposal see section 13.

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# SECTION 7: Handling and storage

## Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

## Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Store in cool place.

## Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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# 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, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

### Respiratory protection

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. 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.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	off-white powder
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	point/range: 125 - 128 °C - lit.
Initial boiling point and boiling range	ca.365 °C at ca.1013,0 hPa - OECD Test Guideline 103
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	ca.0,001 hPa at ca.20 °C - OECD Test Guideline 104
Vapour density	No data available
Relative density	ca.1,53 g/cm <sup>3</sup> at 22 °C -
Water solubility	0,00006 g/l at 20,5 °C - OECD Test Guideline 105 - insoluble
Partition coefficient: n-octanol/water	log Pow: ca.3,2 - OECD Test Guideline 117
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

### Other safety information

Surface tension 72,3 - 72,5 mN/m at 20 °C

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## 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**

No data available

### **Incompatible materials**

Oxidizing agents

### **Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Hydrogen bromide gas

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

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## **SECTION 11: Toxicological information**

### **Information on toxicological effects**

#### **Acute toxicity**

LD50 Oral - Rat - male and female - > 2.000 mg/kg

(OECD Test Guideline 401)

#### **Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation (OECD Test Guideline 404)

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation (OECD Test Guideline 405)

#### **Respiratory or skin sensitization**

- Guinea pig

Result: May cause sensitization by skin contact. (OECD Test Guideline 406)

#### **Germ cell mutagenicity**

Ames test

S. typhimurium 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: Not available

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

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## SECTION 12: Ecological information

### Toxicity

#### Toxicity to fish

static test NOEC - *Oncorhynchus mykiss* (rainbow trout) - 0,21 mg/l

#### Toxicity to daphnia and other aquatic invertebrates

- 96 h

(OECD Test Guideline 203)

Immobilization NOEC - *Daphnia magna* (Water flea) - 0,18 mg/l - 48 h

(OECD Test Guideline 202)

#### Toxicity to algae

Growth inhibition NOEC - *Desmodesmus subspicatus* (green algae) - 0,44 mg/l - 72 h

(OECD Test Guideline 201)

#### Toxicity to bacteria

Respiration inhibition EC50 - Sludge Treatment - > 1.000 mg/l - 3 h (OECD Test Guideline 209)

### Persistence and degradability

Biodegradability aerobic - Exposure time 29 d

Result: - Not biodegradable. (OECD Test Guideline 301B)

### 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

Very toxic to aquatic life with long lasting effects.

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## SECTION 13: Disposal considerations

### Waste treatment methods

### Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. 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.

### **Contaminated packaging**

Dispose of as unused product.

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## **SECTION 14: Transport information**

### **UN number**

ADR/RID: 3077 IMDG: 3077 IATA: 3077

### **UN proper shipping name**

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (4'-Bromomethyl-[1,1'-biphenyl]-2-carbonitrile)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (4'-Bromomethyl-[1,1'-biphenyl]-2-carbonitrile)

IATA: Environmentally hazardous substance, solid, n.o.s. (4'-Bromomethyl-[1,1'- biphenyl]-2-carbonitrile)

### **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. Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

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## **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**

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/>  
Chemical Book



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

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

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

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

EC Inventory:Not Listed.

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

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## 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](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.