

Chemical Safety Data Sheet MSDS / SDS

3-CYANOENZYLZINC BROMIDE

Revision Date:2026-05-31 Revision Number:1

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

Product name : 3-CYANOENZYLZINC BROMIDE
CBnumber : CB8748067
CAS : 117269-72-4
Synonyms : 3-Cyanobenzylzinc bromide solution

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

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

P370+P378 In case of fire: Use ... for extinction.

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

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

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

Hazard statements

H351 Suspected of causing cancer

H335 May cause respiratory irritation

H319 Causes serious eye irritation

H302 Harmful if swallowed

SECTION 3: Composition/information on ingredients

Substance

Product name	: 3-CYANOBENZYLZINC BROMIDE
Synonyms	: 3-Cyanobenzylzinc bromide solution
CAS	: 117269-72-4
MF	: C ₈ H ₆ BrNZn
MW	: 261.43

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

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

If inhaled

After inhalation: fresh air. Call in physician.

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. Call in ophthalmologist. Remove contact lenses.

If swallowed

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

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

4.4 Notes to physician

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

Water Foam

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Hydrogen bromide gas

Zinc/zinc oxides

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

May not get in touch with: Water

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

Forms explosive mixtures with air at ambient temperatures.

5.3 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.

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.

SECTION 6: Accidental release measures

6.1 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.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 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.

Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Keep workplace dry. Do not allow product to come into contact with water.

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

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Never allow product to get in contact with water during storage.

Storage stability Recommended storage temperature

2 - 8 °C

Store under inert gas. Dry residue is explosive. Test for peroxide formation periodically and before distillation. Test for peroxide formation periodically and before distillation.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

['Component', 'CAS-No.', 'Value', 'Control parameters', 'Basis']	['Tetrahydrofuran', '109-99-9', 'PC-TWA', '300 mg/m3', 'Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.']
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Biological occupational exposure limits

['Component', 'CAS-No.', 'Parameters', 'Value', 'Biological specimen', 'Basis']	['Tetrahydrofuran', '109-99-9', 'Tetrahydrofuran', '2 mg/l', 'Urine', 'ACGIH - Biological Exposure Indices (BEI)']	['', 'Remarks', 'End of shift (As soon as possible after exposure ceases)', 'None, None, None']
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8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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

required

Body Protection

Flame retardant antistatic 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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	liquid
b) Color	No data available
c) Odor	No data available
d) Melting point/freezing point	No data available
e) Initial boiling point and boiling range	65.0 - 67.0 °C
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	Upper explosion limit: 11.8 %(V) Lower explosion limit: 1.8 %(V)
h) Flash point	-17 °C - closed cup
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	No data available
p) Density	0.966 g/cm ³ at 25 °C
Relative density	0.966 g/mL at 25 °C
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	Not classified as explosive.
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Chemical stability

sensitive to moisture

10.2 Possibility of hazardous reactions

A risk of explosion and/or of toxic gas formation exists with the following substances: alkali hydroxides

Bromine hydrides

Potassium lithium aluminium hydride thionyl chloride

Oxidizing agents

Oxygen aminophenol with

Peroxides

Exothermic reaction with:

Acids halides peroxi compounds

10.3 Conditions to avoid

Warming.

Moisture.

10.4 Incompatible materials

rubber, various plastics, TinOxidizing agents, Oxygen

10.5 Hazardous decomposition products

Peroxides

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture Acute toxicity

Acute toxicity estimate Oral - 2,038 mg/kg (Calculation method)

Symptoms: Possible symptoms:;, mucosal irritations, Cough, Shortness of breath, Possible damages:;, damage of respiratory tract

Dermal: No data available

Skin corrosion/irritation

Classified based on available data. For more details, see section 2

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye irritation.

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Evidence of a carcinogenic effect.

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Mixture may cause respiratory irritation.

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

Central nervous system depression, Cough, chest pain, Difficulty in breathing, Exposure to high airborne concentrations can cause anesthetic effects., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Components Tetrahydrofuran

Acute toxicity

LD50 Oral - Rat - male and female - 1,650 mg/kg

Remarks: (ECHA)

Symptoms: Irritation of mucous membranes

LC50 Inhalation - Rat - male and female - 6 h - > 14.7 mg/l - vapor (US-EPA)

LD50 Dermal - Rat - male and female - > 2,000 mg/kg (OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 72 h (Draize Test)

Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.

Remarks: (IUCLID)

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

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative (OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female - Red blood cells (erythrocytes)

Result: negative

Carcinogenicity

Suspected of causing cancer.

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Central nervous system

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

May cause drowsiness or dizziness.

Acute oral toxicity - Irritation of mucous membranes

Specific target organ toxicity - repeated exposure Aspiration hazard

Classified based on available data. For more details, see section 2

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

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

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components Tetrahydrofuran

Toxicity to fish flow-through test LC50 - Pimephales promelas (fathead minnow) - 2,160 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to daphnia static test EC50 - Daphnia magna (Water flea) - 3,485 mg/l - and other aquatic 48 h invertebrates (OECD Test Guideline 202)

Toxicity to flow-through test NOEC - Pimephales promelas (fathead fish(Chronic toxicity) minnow) - 216 mg/l - 33 d

Remarks: (ECHA)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 2056

IMDG: 2056

IATA-DGR: 2056

14.2 UN proper shipping name

ADR/RID: TETRAHYDROFURAN,SOLUTION

IMDG: TETRAHYDROFURAN,SOLUTION

IATA-DGR: Tetrahydrofuran,SOLUTION

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA-DGR: 3

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA-DGR: II

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

14.7 Incompatible materials

rubber, various plastics, TinOxidizing agents, Oxygen

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulatory information

Law on the Prevention and Control of Occupational Diseases

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals : Listed

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number : B1A222232745

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

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

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

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.