

SAFETY DATA SHEETS

According to the UN GHS revision 10

1: Identification

1.1 GHS Product identifier

Product name 4,4'-(1H-1,3,4-Triazol-1-ylmethylene)dibenzonitrile

1.2 Other means of identification

Product number 112809-52-6

Other names 4,4'-(1H-1,3,4-Triazol-1-ylmethylene)dibenzonitrile

1.3 Recommended use of the chemical and restrictions on use

Identified uses Industrial and scientific research use.

Uses advised against no data available

1.4 Supplier's details

Company Zhongshan Greenrock Technology Co., Ltd.

Address No. 138, Jinsan Avenue, Sanjiao Town, Zhongshan City, Guangdong Province, China

Telephone +86-2087066781

1.5 Emergency phone number

Emergency phone number +86-2087066781

Service hours Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

2: Hazard identification

2.1 Emergency Overview

Substances with long-term health risks may cause cancer, gene mutations, or reproductive system damage. Even short-term exposure may have long-term health effects and exposure must be strictly controlled.

2.2 GHS Classification

Reproductive toxicity : Category 2

Specific target organ toxicity, repeated exposure : Category 2

2.3 GHS label elements, including precautionary statements

Pictogram(s)**Signal word**

Warning

Hazard statement(s)

H361fd Suspected of damaging fertility; Suspected of damaging the unborn child

H373 May causes damage to organs through prolonged or repeated exposure

Precautionary statement(s)**Prevention**

P203 Obtain, read and follow all safety instructions before use.

P260 Do not breathe dust/fume/gas/mist/vapors/spray.

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

Response

P318 if exposed or concerned, get medical advice.

P319 Get medical help if you feel unwell.

Storage

P405 Store locked up.

Disposal

P501 Dispose of contents/container to ...

2.4 Physical and chemical

Although they may not be immediately dangerous, some substances may also be irritants or corrosives. They may decompose and produce more toxic products during long-term storage.

2.5 Health hazards

Carcinogenicity, Long-term exposure may increase the risk of cancer. Mutagenicity: May cause genetic damage, affecting offspring. Reproductive toxicity: May affect fertility or cause fetal malformations. Symptoms typically appear after a latent period of several years.

2.6 Environmental hazards

May persist and accumulate in the environment. Chronic toxicity to aquatic and terrestrial organisms can affect their reproductive capacity. It may accumulate through the food chain, ultimately affecting human health.

2.7 Other hazards which do not result in classification

no data available

3: Composition/information on ingredients**3.1 Substances**

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
4,4'-(1H-1,3,4-Triazol-1-ylmethylene)dibenzonitrile	4,4'-(1H-1,3,4-Triazol-1-ylmethylene)dibenzonitrile	112809-52-6	-	99%

4: First-aid measures

4.1 General advice

Stop contact immediately and remove contaminated clothing (rinse with clean water and then wash); wash skin with soap and water, record contact history (including contact time and frequency); and have regular physical examinations (such as chest CT and blood routine once a year).

4.2 If inhaled

Move to fresh air. If carcinogenic gases (such as benzene) are inhaled and coughing or chest tightness occurs, seek medical attention. Those with long-term exposure need to monitor lung function and blood routine.

4.3 In case of skin contact

Rinse with soap and running water for 15 minutes. If skin is irritated, apply a non-irritating moisturizer; avoid breaking the skin to prevent penetration of substances.

4.4 In case of eye contact

Rinse with saline for 10 minutes and then instill artificial tears; if discomfort persists, seek medical attention from an ophthalmologist.

4.5 If swallowed

Do not induce vomiting, seek medical attention immediately, and bring the substance's SDS; inform the doctor of the substance's carcinogenic/mutagenic properties and perform a gastrointestinal endoscopy if necessary.

4.6 Most important symptoms and effects, both acute and delayed

Acute symptoms: mild skin/eye irritation; long-term effects: carcinogenicity (such as lung cancer, leukemia), mutagenicity (chromosomal abnormalities), reproductive toxicity (infertility, fetal malformations).

4.7 Protection of first-aiders

Rescuers need to wear chemical protective clothing, gas masks (equipped with organic vapor filter cartridges), and chemical protective gloves; equipment must be thoroughly cleaned after contact to avoid residue.

4.8 Notes to physician

Inform the doctor of the substance name and exposure history; long-term exposure requires a special physical examination plan (such as blood tests every 6 months and tumor markers every year)

5: Fire-fighting measures

5.1 Unsuitable extinguishing media

It is strictly forbidden to use fire extinguishing agents that may cause the spread of toxic substances (such as high-pressure water jets); if it contains flammable ingredients, avoid using carbon dioxide (concentrated toxic vapor).

5.2 Specific hazards during fire fighting

Combustion releases carcinogenic/mutagenic gases (such as benzopyrene and formaldehyde), which are harmful to health if exposed for a long time. The combustion products of some substances are easily adsorbed on dust, expanding the scope of pollution. Toxic substances are not easy to decompose and require professional handling after fire extinguishing.

5.3 Hazardous combustion products

Polycyclic aromatic hydrocarbons (carcinogenic), formaldehyde (mutagenic), heavy metal smoke (such as chromium, nickel), chlorides (when containing chlorine).

5.4 Specific extinguishing methods

Small area: Use dry powder/foam to extinguish the fire, and use water mist to dilute the toxic vapor; Large area: Evacuate personnel, if fire must be extinguished, cover with foam (to reduce vapor release); After extinguishing the fire, conduct toxicity testing on the area and dispose of pollutants as hazardous waste.

5.5 Special protective equipment for fire-fighters

Wear chemical protective clothing, positive pressure air respirator, and chemical protective gloves; carry a toxic gas detector (to detect benzene, formaldehyde, etc.); wear a dust mask (to protect against toxic dust) during work, and conduct a health check after work.

6: Accidental release measures

6.1 Protective measures for workers

Wear fully enclosed chemical protective clothing, positive pressure respirator (volatile), toxic-resistant gloves + goggles; workers should undergo regular physical examinations and record their exposure history; eating, drinking and smoking are prohibited.

6.2 Environmental protection measure

Isolate the contaminated area within 20 meters and conduct long-term environmental monitoring (soil/air); leaks are prohibited from being discarded at will; the contaminated area must be released after passing the inspection by the environmental protection department.

6.3 Containment methods for leaked chemicals

Liquids should be collected in disposable corrosion-resistant containers (marked with hazard categories); solids should be collected in chemical-resistant bags (to prevent dust); and stored separately in dedicated hazardous waste warehouses.

6.4 Cleanup methods for chemical spills

Small leakage: absorbed by special adsorption materials and then packaged in chemical-proof bags; large leakage: transferred by professional team using special equipment; after cleaning, the ground is treated with disinfectant.

6.5 Measures to prevent the spread of leaks

20-meter isolation zone + warning signs; high-efficiency filtration and ventilation (volatile); chemical isolation belt to prevent spread to residential areas.

6.6 Container leakage treatment

Minor leaks: seal with professional sealant + tightness test; serious leaks: evacuate, transfer by professional team, and dispose of the container as hazardous waste.

6.7 Special considerations

Operators need special training; protective equipment must be disinfected and tested before reuse; leak handling must be reported to the environmental protection department.

7: Handling and storage

7.1 Safe storage conditions

Stored in a closed, leak-proof warehouse (walls lined with polyethylene film and floors with impermeable resin); containers are made of non-degradable materials (such as high-density polyethylene, borosilicate glass) with anti-theft lids (requires a key to open); the warehouse is equipped with an air purification system (HEPA filter, filtration efficiency >99.97%).

7.2 Storage precautions

Isolate from children and unrelated personnel, and place biohazard signs at the warehouse entrance; store separately to avoid mixing with other chemicals; test the concentration of hazardous substances in the warehouse every quarter to ensure that it is below the occupational exposure limit (such as carcinogen OEL > 0.01mg/m³); discarded containers must be sterilized at high temperature (>121°, 30 minutes) before disposal.

7.3 VCI Storage Grade

Level 4 (lowest): Metal containers are treated with ordinary anti-rust treatment (such as galvanizing, thickness > 10µm) and corrosion is checked once a year; the humidity in the warehouse is controlled at 45%-65% to avoid damage to the containers due to moisture.

7.4 Recommended storage temperature

Store at 10-30°C, away from light (e.g., some photosensitive carcinogens must be stored in brown containers); easily degradable substances (e.g., some organic carcinogens) must be stored at >25°C, equipped with light-proof and sun-shading facilities; long-term storage (over 1 year) requires the stability of the substance to be checked every 3 months (if the label has a recommended storage temperature, follow the label).

7.5 Handling

For precautions see Safety Data Sheet section 2

Advice on safe handling : Work under hood. Do not inhale substance/mixture.

8: Exposure controls/personal protection

8.1 Respiratory protection

When exposed to carcinogens (such as benzene and formaldehyde) for a long time, wear a powered air-purifying respirator (APF?50); dust (such as asbestos) requires Type P100 filter cotton to ensure no leakage.

8.2 Recommended Filter type

For organic carcinogens, choose Type A2 filter cartridge; for inorganic carcinogenic gases (such as arsine), choose Type E+K composite filter cartridge; for dust, choose Type P100 filter cotton.

8.3 Eye/face protection

Wear chemical protection goggles + protective mask. The mask material should be resistant to toxic penetration. The lenses need to be replaced regularly for long-term work (to prevent aging).

8.4 Skin and body protection

Wear impermeable chemical protective clothing made of polyethylene + aluminum foil coating (anti-organic vapor penetration); avoid skin damage during operation to prevent material intrusion.

8.5 Hand protection

Wear toxic and chemical-resistant gloves made of butyl rubber or fluororubber. Gloves need to be regularly tested for penetration (once every three months) and replaced immediately if unqualified.

8.6 Hygiene measures

After work, clean the skin with a special detergent (such as a neutral surfactant), then rinse with running water for 10 minutes; clothes must be washed separately and must not be mixed with household clothes; undergo special physical examinations every year (such as chest CT, chromosome examination).

9: Physical and chemical properties and safety characteristics

Physical state	no data available
Colour	no data available
Odour	no data available
Melting point/freezing point	239-243 °C
Boiling point or initial boiling point and boiling range	563.5oC at 760mmHg
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available

Flash point	294.6oC
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Chloroform (Slightly, Heated), Methanol (Slightly)
Partition coefficient n-octanol/water	no data available
Vapour pressure	1.01E-12mmHg at 25°C
Density and/or relative density	1.21g/cm3
Relative vapour density	no data available
Particle characteristics	no data available

10: Stability and reactivity

10.1 Reactivity

no data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

no data available

11: Toxicological information

11.1 Acute toxicity

Oral: no data available

Inhalation: no data available

Dermal: no data available

11.2 Skin corrosion/irritation

no data available

11.3 Serious eye damage/irritation

no data available

11.4 Respiratory or skin sensitization

no data available

11.5 Germ cell mutagenicity

no data available

11.6 Carcinogenicity

no data available

11.7 Reproductive toxicity

no data available

11.8 STOT-single exposure

no data available

11.9 STOT-repeated exposure

no data available

11.10 Aspiration hazard

no data available

12: Ecological information

12.1 Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: 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 Other adverse effects

no data available

13: Disposal considerations

13.1 Disposal methods for waste chemicals

It must be handled by an organization with hazardous waste disposal qualifications, with high-temperature incineration (temperature $\geq 900^{\circ}\text{C}$) being preferred to completely destroy hazardous substances. Waste that cannot be incinerated must be chemically degraded or stabilized before being safely landfilled. Contaminated containers must be sterilized at high temperatures or chemically before disposal.

13.2 Precautions

Disposal personnel must wear special protective equipment and undergo regular health checks; waste must be tightly sealed to prevent leakage; waste gas and wastewater generated during the disposal process must undergo special treatment to ensure compliance with standards; disposal records must be kept for a long time (at least 30 years); and mixing with ordinary waste is prohibited.

14: Transport information

14.1 UN Number

ADR/RID: no data available

IMDG: no data available

IATA: no data available

14.2 UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

14.3 Transport hazard class(es)

ADR/RID: no data available

IMDG: no data available

IATA: no data available

14.4 Packing group, if applicable

ADR/RID: no data available

IMDG: no data available

IATA: no data available

14.5 Environmental hazards

ADR/RID: no

IMDG: no

IATA: no

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
4,4'-(1H-1,3,4-Triazol-1-ylmethylene)dibenzonitrile	4,4'-(1H-1,3,4-Triazol-1-ylmethylene)dibenzonitrile	112809-52-6	
New Zealand Inventory of Chemicals (NZIoC)			Not Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Not Listed.
Vietnam National Chemical Inventory			Not Listed.
Australian Inventory of Industrial Chemicals (AIIC)			Not Listed.
Catalogue of Strictly Restricted Toxic Chemicals in China			Not Listed.
China Catalog of Hazardous chemicals 2015			Not Listed.
European INventory of Existing Commercial chemical Substances			Not Listed.
IARC Monographs on the Evaluation of Carcinogenic Risks to Humans			Not Listed.
TSCA Inventory of Chemical Substances			Not Listed.

16: Other information

Information on revision

SDS Creation Date July 1, 2025

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Abbreviations and acronyms in SDS

- 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%

SDS References

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Any questions regarding this Safety Data Sheet, Please send your inquiry to sales@MolBest.com

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