

## Chemical Safety Data Sheet MSDS / SDS

**3,3'-Dimethyl-4,4'-biphenylene diisocyanate**Revision Date:2025-07-19 Revision Number:1

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

Product name : 3,3'-Dimethyl-4,4'-biphenylene diisocyanate  
CBnumber : CB2485599  
CAS : 91-97-4  
EINECS Number : 202-112-7  
Synonyms : TODI,3,3'-Dimethyl-4,4'-biphenylene diisocyanate

**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

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**SECTION 2: Hazards identification****Classification of the substance or mixture**

Skin sensitization, Sub-category 1A  
Acute toxicity - Category 4, Inhalation  
Respiratory sensitization, Category 1  
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

**Label elements****Pictogram(s)**

Signal word : Danger

**Hazard statement(s)**

H315 Causes skin irritation  
H319 Causes serious eye irritation  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled  
H341 Suspected of causing genetic defects

### Precautionary statement(s)

P201 Obtain special instructions before use.

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

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

P264 Wash hands thoroughly after handling.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P271 Use only outdoors or in a well-ventilated area.

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

P284 Wear respiratory protection.

P308+P313 IF exposed or concerned: Get medical advice/attention.

P405 Store locked up.

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

### Prevention

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

P272 Contaminated work clothing should not be allowed out of the workplace.

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

P271 Use only outdoors or in a well-ventilated area.

P284 [In case of inadequate ventilation] wear respiratory protection.

P273 Avoid release to the environment.

### Response

P302+P352 IF ON SKIN: Wash with plenty of water/...

P333+P317 If skin irritation or rash occurs: Get medical help.

P321 Specific treatment (see ... on this label).

P362+P364 Take off contaminated clothing and wash it before reuse.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P317 Get medical help.

P342+P316 If experiencing respiratory symptoms: Get emergency medical help immediately.

P391 Collect spillage.

### Storage

none

### Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

### Other hazards

no data available

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## SECTION 3: Composition/information on ingredients

### Substance

Product name : 3,3'-Dimethyl-4,4'-biphenylene diisocyanate

|           |   |
|-----------|---|
| Synonyms  | : TODI,3,3'-Dimethyl-4,4'-biphenylene diisocyanate              |
| CAS       | : 91-97-4   |
| EC number | : 202-112-7   |
| MF        | : C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> |
| MW        | : 264.28  |

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## SECTION 4: First aid measures

### Description of first aid measures

#### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately.

Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

### Most important symptoms and effects, both acute and delayed

Excerpt from ERG Guide 155 [Substances - Toxic and/or Corrosive (Flammable / Water-Sensitive)]: TOXIC; inhalation, ingestion or contact (skin, eyes) with vapors, dusts or substance may cause severe injury, burns or death. Bromoacetates and chloroacetates are extremely irritating/lachrymators. Reaction with water or moist air will release toxic, corrosive or flammable gases. Reaction with water may generate much heat that will increase the concentration of fumes in the air. Fire will produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution. (ERG, 2016)

### Indication of any immediate medical attention and special treatment needed

no data available

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## SECTION 5: Firefighting measures

### Extinguishing media

Excerpt from ERG Guide 155 [Substances - Toxic and/or Corrosive (Flammable / Water-Sensitive)]: Note: Most foams will react with the material and release corrosive/toxic gases. CAUTION: For Acetyl chloride (UN1717), use CO<sub>2</sub> or dry chemical only. SMALL FIRE: CO<sub>2</sub>, dry chemical, dry sand, alcohol-resistant foam. LARGE FIRE: Water spray, fog or alcohol-resistant foam. FOR CHLOROSILANES, DO NOT USE WATER; use AFFF alcohol-resistant medium-expansion foam. Move containers from fire area if you can do it without risk. Use water spray or fog; do not use straight streams. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Do not get water inside containers. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. (ERG, 2016)

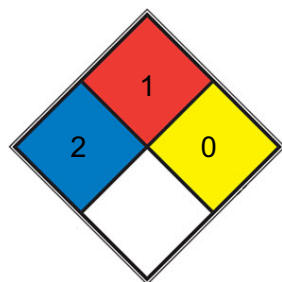
### Specific Hazards Arising from the Chemical

Excerpt from ERG Guide 155 [Substances - Toxic and/or Corrosive (Flammable / Water-Sensitive)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapors may travel to source of ignition and flash back. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Substance will react with water (some violently) releasing flammable, toxic or corrosive gases and runoff. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated or if contaminated with water. (ERG, 2016)

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 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, [N2](#))

**SPEC.**  
**HAZ.**

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### Environmental precautions

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

### Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

## SECTION 7: Handling and storage

### Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

### Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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## SECTION 8: Exposure controls/personal protection

### Control parameters

#### Occupational Exposure limit values

no data available

#### Biological limit values

no data available

### Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### Individual protection measures

#### Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

#### Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

#### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

#### Thermal hazards

no data available

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

|  |  |
|--|--|
| Physical state   | Solid. Pellets.                                      |
| Colour   | White - yellowish.                                   |
| Odour  | no data available                                    |
| Melting point/freezing point                             | $\geq 71.6$ - $\leq 72$ °C. Atm. press.: 1021.9 hPa. |
| Boiling point or initial boiling point and boiling range | Atm. press.: 101.42 kPa.                             |

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|  |   |
|--|---|
| Flammability                                       | no data available   |
| Lower and upper explosion limit/flammability limit | no data available   |
| Flash point  | 15°C(lit.)  |
| Auto-ignition temperature                          | Remarks:No self-ignition observed up to the melting point.  |
| Decomposition temperature                          | no data available   |
| pH   | no data available   |
| Kinematic viscosity                                | no data available   |
| Solubility   | In water: 0.594 mg/L. Temperature:25 °C. Remarks:The substance is not within the applicability domain of the model. |
| Partition coefficient n-octanol/water              | log Pow = 4.5. Temperature:20 °C. Remarks:No information about pH value available.                                  |
| Vapour pressure                                    | 0 Torr. Temperature:25 °C. Remarks:Corresponding to 2.85 E-5 mbar (conversion: 760 torr = 1.013 bar).               |
| Density and/or relative density                    | 1.331 dimensionsless. Temperature:20 °C.  |
| Relative vapour density                            | no data available   |
| Particle characteristics                           | no data available   |

## SECTION 10: Stability and reactivity

### Reactivity

No rapid reaction with air. No rapid reaction with water.

### Chemical stability

no data available

### Possibility of hazardous reactions

Isocyanates and thioisocyanates, such as 3,3'-DIMETHYL-4,4'-DIPHENYLENE DIISOCYANATE, are incompatible with many classes of compounds, reacting exothermically to release toxic gases. Reactions with amines, aldehydes, alcohols, alkali metals, ketones, mercaptans, strong oxidizers, hydrides, phenols, and peroxides can cause vigorous releases of heat. Acids and bases initiate polymerization reactions in these materials. Some isocyanates react with water to form amines and liberate carbon dioxide. Base-catalysed reactions of isocyanates with alcohols should be carried out in inert solvents. Such reactions in the absence of solvents often occur with explosive violence, [Wischmeyer(1969)].

### Conditions to avoid

no data available

### Incompatible materials

no data available

### Hazardous decomposition products

no data available

## SECTION 11: Toxicological information

### **Acute toxicity**

- Oral: no data available
- Inhalation: no data available
- Dermal: LD50 - rat (male/female) - > 2 000 mg/kg bw.

### **Skin corrosion/irritation**

no data available

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

no data available

### **Respiratory or skin sensitization**

no data available

### **Germ cell mutagenicity**

no data available

### **Carcinogenicity**

no data available

### **Reproductive toxicity**

no data available

### **STOT-single exposure**

no data available

### **STOT-repeated exposure**

no data available

### **Aspiration hazard**

no data available

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## **SECTION 12: Ecological information**

### **Toxicity**

Toxicity to fish: LC50 - *Oncorhynchus mykiss* (previous name: *Salmo gairdneri*) - 0.25 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - > 1.2 mg/L - 48 h.

Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - > 4 mg/L - 72 h.

Toxicity to microorganisms: EC50 - activated sludge, domestic - > 1 000 mg/L - 3 h.

### **Persistence and degradability**

no data available

### **Bioaccumulative potential**

no data available

### **Mobility in soil**

no data available

### **Other adverse effects**

no data available

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## **SECTION 13: Disposal considerations**

### **Disposal methods**

#### **Product**

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

#### **Contaminated packaging**

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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## **SECTION 14: Transport information**

### **UN Number**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **UN Proper Shipping Name**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Transport hazard class(es)**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Packing group, if applicable**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Environmental hazards**



ADR/RID: Yes

IMDG: Yes

IATA: Yes

### **Special precautions for user**

no data available

### **Transport in bulk according to IMO instruments**

no data available

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## **SECTION 15: Regulatory information**

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

#### **European Inventory of Existing Commercial Chemical Substances (EINECS)**

Listed.

#### **EC Inventory**

Listed.

#### **United States Toxic Substances Control Act (TSCA) Inventory**

Listed.

#### **China Catalog of Hazardous chemicals 2015**

Not Listed.

#### **New Zealand Inventory of Chemicals (NZIoC)**

Not Listed.

#### **PICCS**

Not Listed.

#### **Vietnam National Chemical Inventory**

Listed.

#### **IECSC**

Not Listed.

#### **Korea Existing Chemicals List (KECL)**

Listed.

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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

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](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/>

### 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.