

## Chemical Safety Data Sheet MSDS / SDS

**1,3-BIS(2-ISOCYANATO-2-PROPYL)BENZENE**Revision Date:2024-12-21 Revision Number:1

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

Product name : 1,3-BIS(2-ISOCYANATO-2-PROPYL)BENZENE  
CBnumber : CB3496112  
CAS : 2778-42-9  
EINECS Number : 220-474-4  
Synonyms : TMXDI,1,3-Bis(2-isocyanato-2-propyl)benzene

**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

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

Skin irritation, Category 2  
Skin sensitization, Sub-category 1A  
Eye irritation, Category 2  
Acute toxicity - Category 1, Inhalation  
Respiratory sensitization, Category 1  
Specific target organ toxicity – repeated exposure, 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



H317 May cause an allergic skin reaction  
H319 Causes serious eye irritation  
H320 Causes eye irritation  
H330 Fatal if inhaled  
H372 Causes damage to organs through prolonged or repeated exposure  
H400 Very toxic to aquatic life  
H410 Very toxic to aquatic life with long lasting effects

#### **Precautionary statement(s)**

P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P264 Wash hands thoroughly after handling.  
P264 Wash skin thoroughly after handling.  
P271 Use only outdoors or in a well-ventilated area.  
P272 Contaminated work clothing should not be allowed out of the workplace.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P284 Wear respiratory protection.  
P310 Immediately call a POISON CENTER or doctor/physician.  
P391 Collect spillage. Hazardous to the aquatic environment  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P405 Store locked up.  
P403+P233 Store in a well-ventilated place. Keep container tightly closed.  
P501 Dispose of contents/container to.....

#### **Prevention**

P264 Wash ... thoroughly after handling.  
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P272 Contaminated work clothing should not be allowed out of the workplace.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P271 Use only outdoors or in a well-ventilated area.  
P284 [In case of inadequate ventilation] wear respiratory protection.  
P270 Do not eat, drink or smoke when using this product.  
P273 Avoid release to the environment.

#### **Response**

P302+P352 IF ON SKIN: Wash with plenty of water/...  
P321 Specific treatment (see ... on this label).  
P332+P317 If skin irritation occurs: Get medical help.  
P362+P364 Take off contaminated clothing and wash it before reuse.  
P333+P317 If skin irritation or rash occurs: Get medical help.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P316 Get emergency medical help immediately.



P320 Specific treatment is urgent (see ... on this label).

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

P319 Get medical help if you feel unwell.

P391 Collect spillage.

#### **Storage**

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

#### **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	: 1,3-BIS(2-ISOCYANATO-2-PROPYL)BENZENE
Synonyms	: TMXDI, 1,3-Bis(2-isocyanato-2-propyl)benzene
CAS	: 2778-42-9
EC number	: 220-474-4
MF	: C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
MW	: 244.29

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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**

no data available

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

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration,



preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Isocyanates, aliphatic thiocyanates, and related compounds

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## SECTION 5: Firefighting measures

### Extinguishing media

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

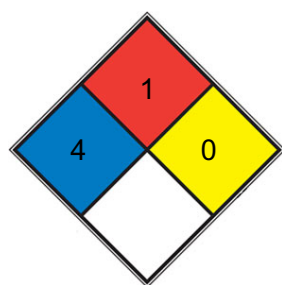
### Specific Hazards Arising from the Chemical

no data available

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### NFPA 704



☒ HEALTH 4 Very short exposure could cause death or major residual injury (e.g. hydrogen cyanide, phosgene, methyl isocyanate, [hydrofluoric acid](#))

☒ 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.

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## 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.

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## 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	Oil
Colour	Colourless
Odour	no data available
Melting point/freezing point	4 °C. Atm. press.:1 atm. Remarks:OECD 102 suggests that melting should be reported as a range marked by onset and endset of melting peak. Hence the melting range of TMXDI is 4-12 °C. However the ASTM method and SOP used states to report the onset as the melt. So the reported m.p. is 4°C.
Boiling point or initial boiling point and boiling range	249.2 °C. Atm. press.:Ca. 1 atm. Remarks:By DSC technique.;249.4 °C. Atm. press.:Ca. 1 atm.
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	168 °C. Atm. press.:1 atm.
Auto-ignition temperature	498 °C. Atm. press.:1 atm.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	dynamic viscosity (in mPa s) = 18.2. Temperature:25.0°C.
Solubility	Chloroform (Slightly)
Partition coefficient n-octanol/water	log Pow = 4.74. Remarks:Data estimated by KOWWIN v1.67 for m-TMXDI; However, as m-TMXDI contains isocyanate groups which rapidly hydrolyse the log Pow QSAR estimation is questionable.;log Pow = 3.53. Remarks:Data estimated by KOWWIN v1.67 for hydrolysed product 1,3-bis(2-{3-[2-(carbamoylamino)propan-2-yl]phenyl}propan-2-yl)urea.;log Pow = 1.89. Remarks:Data estimated by KOWWIN v1.67 for hydrolysed product tetramethyl-m-xylylene diamine.
Vapour pressure	0.003 mm Hg. Temperature:25 °C.
Density and/or relative density	1.07 g/cm <sup>3</sup> . Temperature:25 °C.
Relative vapour density	no data available
Particle characteristics	no data available

## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

no data available

### Possibility of hazardous reactions

no data available

### Conditions to avoid

no data available

### Incompatible materials

no data available



## Hazardous decomposition products

When heated to decomposition it emits toxic vapors of NO<sub>x</sub>.

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## SECTION 11: Toxicological information

### Acute toxicity

- Oral: LD<sub>50</sub> Rat oral 4600 mg/kg
- Inhalation: LD<sub>50</sub> Guinea pig inhalation 240 mg/m<sup>3</sup> for 1 hr
- Dermal: no data available

### 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: LC<sub>50</sub> - *Lepomis macrochirus* - > 65.88 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: LC<sub>50</sub> - *Daphnia magna* - 6.5 mg/L - 24 h.

Toxicity to algae: EC<sub>50</sub> - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - 6.9 mg/L



- 72 h.

Toxicity to microorganisms: EC50 - activated sludge of a predominantly domestic sewage - ca. 140 mg/L - 3 h. Remarks: Respiration rate.

### **Persistence and degradability**

AEROBIC: 1,3-Bis(1-isocyanato-1-methylethyl)benzene was not found to be readily biodegradable by the OECD Closed Bottle Test. A solution of 1,3-bis(1-isocyanato-1-methylethyl)benzene was inoculated with a low concentration of activated sludge from a mixed population and kept in closed bottles in the dark at a constant temperature of 20 deg C. The degradation was followed by oxygen analyses over a 28-day period. A parallel control with inoculum, but without test material, was run as a blank correction factor. The procedure was validated by means of a reference substance (aniline) of known biodegradability. Degradation after 28-days was determined to be 13.7% as compared to 95% for the aniline reference material. Because a level of 70% was not reached, this substance is not "Readily Biodegradable" by this test procedure(2). Due to the rapid hydrolysis of isocyanates, the test probably is for the diamine hydrolysis product(SRC).

### **Bioaccumulative potential**

1,3-Bis(1-isocyanato-1-methylethyl)benzene, similar to most isocyanates(1-4), is expected to hydrolyze in aqueous solution; therefore, bioconcentration will not be environmentally relevant(SRC).

### **Mobility in soil**

1,3-Bis(1-isocyanato-1-methylethyl)benzene, similar to most isocyanates(1-4), is expected to hydrolyze in aqueous solution; therefore, leaching and adsorption to sediment will not be environmentally relevant(SRC).

### **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: no data available

IMDG: no data available

IATA: no data available

### **UN Proper Shipping Name**



ADR/RID: no data available

IMDG: no data available

IATA: no data available

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

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

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

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (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)**

Listed.

#### **PICCS**

Not Listed.

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

Listed.

#### **IECSC**

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?pagelD=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pagelD=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.