

## Chemical Safety Data Sheet MSDS / SDS

**1,3-Bis(isocyanatomethyl)benzene**

Revision Date:2024-07-20 Revision Number:1

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

Product name : 1,3-Bis(isocyanatomethyl)benzene  
CBnumber : CB6158648  
CAS : 3634-83-1  
EINECS Number : 222-852-4  
Synonyms : XDI, 1,3-Bis(isocyanatomethyl)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

**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

**Precautionary statements**

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P284 Wear respiratory protection.  
P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.  
P342+P311 IF experiencing respiratory symptoms: call a POISON CENTER or doctor/physician.

**Hazard statements**

H226 Flammable liquid and vapour

H314 Causes severe skin burns and eye damage

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: 1,3-Bis(isocyanatomethyl)benzene
Synonyms	: XDI, 1,3-Bis(isocyanatomethyl)benzene
CAS	: 3634-83-1
EC number	: 222-852-4
MF	: C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>
MW	: 188.18

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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

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

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Do NOT induce vomiting. 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 cyanide (hydrocyanic acid)

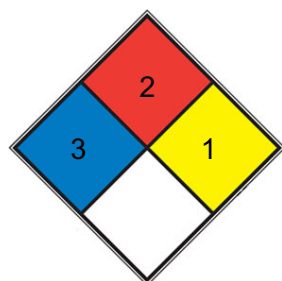
## Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

## Further information

Use water spray to cool unopened containers.

## NFPA 704



☒ HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

☒ FIRE 2 Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

☒ REACT 1 Normally stable, but can become unstable at elevated temperatures and pressures (e.g. [propene](#))

☐ SPEC.

☐ HAZ.

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition.

Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

### Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet- brushing and place in container for disposal according to local regulations (see section 13).

### Reference to other sections

For disposal see section 13.

## SECTION 7: Handling and storage

## Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

## Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Recommended storage temperature 2 - 8 °C

Light sensitive. Store under inert gas. Moisture sensitive. Exposure to moisture.

## 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

Tightly fitting safety goggles. Faceshield (8-inch minimum). 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.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested: Dermatrill? (KCL 740 / Aldrich Z677272, Size M)

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: Dermatrill? (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific

situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

#### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. 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.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	light yellow liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	-7°C
Initial boiling point and boiling range	88 - 90 °C at 0,03 hPa
Flash point	42 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	1,202 g/mL at 20 °C
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
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

No data available

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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

Heat, flames and sparks.

## Incompatible materials

Amines, Alcohols

## Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Hydrogen cyanide (hydrocyanic acid)

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 - 5.350 mg/kg

### Skin corrosion/irritation

Skin - Rabbit

Result: Severe skin irritation

### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Severe eye irritation

### Respiratory or skin sensitization Germ cell mutagenicity

No data available

### 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: NR0147000

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## SECTION 12: Ecological information

### **Toxicity**

No data available

### **Persistence and degradability**

No data available

### **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**

No data available

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## SECTION 13: Disposal considerations

### **Waste treatment methods**

#### **Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

#### **Contaminated packaging**

Dispose of as unused product.

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## SECTION 14: Transport information

### **UN number**

ADR/RID: 2920 IMDG: 2920 IATA: 2920

### **UN proper shipping name**

ADR/RID: CORROSIVE LIQUID, FLAMMABLE, N.O.S. (1,3-Bis(isocyanatomethyl)benzene) IMDG: CORROSIVE LIQUID, FLAMMABLE, N.O.S. (1,3-Bis(isocyanatomethyl)benzene) IATA: Corrosive liquid, flammable, n.o.s. (1,3-Bis(isocyanatomethyl)benzene)

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

ADR/RID: 8 (3) IMDG: 8 (3) IATA: 8 (3)

### **Packaging group**

ADR/RID: II IMDG: II IATA: II

### **Environmental hazards**

ADR/RID: no IMDG Marine pollutant: no IATA: no

### **Special precautions for user**

No data available

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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**

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

EC Inventory:Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

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

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## **SECTION 16: Other information**

### **Abbreviations and acronyms**

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

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average



## 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.