

## Chemical Safety Data Sheet MSDS / SDS

**3,5-BIS(TRIFLUOROMETHYL)PHENYL ISOCYANATE**

Revision Date:2023-12-07 Revision Number:1

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

Product name : 3,5-BIS(TRIFLUOROMETHYL)PHENYL ISOCYANATE  
CBnumber : CB5275483  
CAS : 16588-74-2  
Synonyms : 1-isocyanato-3,5-bis(trifluoromethyl)benzene,3,5-bis(trifluoromethyl)phenyl isocyanate

**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

Warning

**Precautionary statements**

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

P405 Store locked up.

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

P310 Immediately call a POISON CENTER or doctor/physician.

P309 IF exposed or if you feel unwell:

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.

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

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

P264 Wash skin thoroughly after handling.

P264 Wash hands thoroughly after handling.  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

#### **Hazard statements**

H335 May cause respiratory irritation  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled  
H332 Harmful if inhaled  
H331 Toxic if inhaled  
H319 Causes serious eye irritation  
H315 Causes skin irritation  
H312 Harmful in contact with skin  
H302 Harmful if swallowed  
H227 Combustible liquid

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name : 3,5-BIS(TRIFLUOROMETHYL)PHENYL ISOCYANATE  
Synonyms : 1-isocyanato-3,5-bis(trifluoromethyl)benzene,3,5-bis(trifluoromethyl)phenyl isocyanate  
CAS : 16588-74-2  
MF : C9H3F6NO  
MW : 255.12

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## SECTION 4: First aid measures

### **Description of first aid measures**

#### **General advice**

Consult a physician. Show this 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**

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

Small (incipient) fires must be extinguished with alcohol resistant foam, dry chemical powder or carbon dioxide. Large amounts of water are ineffective. Cool containers with large amounts of water.

#### Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Hydrogen fluoride

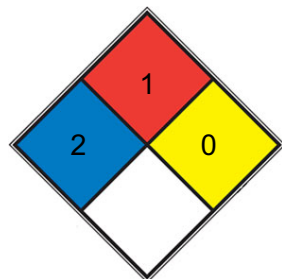
#### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### Further information

Use water spray to cool unopened containers.

#### 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, [N<sub>2</sub>](#))

SPEC.

HAZ.

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## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

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

Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours 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). Keep in suitable, closed containers for disposal.

## **Reference to other sections**

For disposal see section 13.

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# SECTION 7: Handling and storage

## **Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour 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.

Moisture sensitive.

## **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**

Face shield and safety glasses 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.

#### Body Protection

Complete suit protecting against chemicals, 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	liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	No data available
Initial boiling point and boiling range	62 °C (2 mmHg)
Flash point	68 °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	1,476 g/cm <sup>3</sup> at 25 °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. Extremes of temperature and direct sunlight.

## **Incompatible materials**

Strong oxidizing agents

## **Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Hydrogen fluoride

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**

No data available

### **Skin corrosion/irritation**

No data available

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

No data available

### **Respiratory or skin sensitisation Germ cell mutagenicity**

No data available

### **Carcinogenicity**

IARC: No component 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**

Inhalation - May cause respiratory irritation.

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

### **Additional Information**

RTECS: Not available

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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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**

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

### **Other adverse effects**

No data available

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## SECTION 13: Disposal considerations

### **Waste treatment methods**

### **Product**

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

### **Contaminated packaging**

Dispose of as unused product.

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## SECTION 14: Transport information

### **UN number**

ADR/RID: 2206 IMDG: 2206 IATA: 2206

### **UN proper shipping name**

ADR/RID: ISOCYANATES, TOXIC, N.O.S. (3,5-Bis(trifluoromethyl)phenyl isocyanate) IMDG: ISOCYANATES, TOXIC, N.O.S. (3,5-Bis(trifluoromethyl)phenyl isocyanate) IATA: Isocyanates, toxic, n.o.s. (3,5-Bis(trifluoromethyl)phenyl isocyanate)

## Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

## Packaging group

ADR/RID: III IMDG: III IATA: III

## 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

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

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

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

EC Inventory:Not Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

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

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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.