

Chemical Safety Data Sheet MSDS / SDS

4-Chloro-3-(trifluoromethyl)phenyl isocyanate

Revision Date:2024-11-23 Revision Number:1

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

Product identifier

| | |
|---------------|---|
| Product name | : 4-Chloro-3-(trifluoromethyl)phenyl isocyanate |
| CBnumber | : CB8262374 |
| CAS | : 327-78-6 |
| EINECS Number | : 000-000-0 |
| Synonyms | : 4-CHLORO-3-(TRIFLUOROMETHYL)PHENYL ISOCYANATE, 1-chloro-4-isocyanato-2-(trifluoromethyl)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

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.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P284 Wear respiratory protection.

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.

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

SECTION 3: Composition/information on ingredients

Substance

| | |
|--------------|---|
| Product name | : 4-Chloro-3-(trifluoromethyl)phenyl isocyanate |
| Synonyms | : 4-CHLORO-3-(TRIFLUOROMETHYL)PHENYL ISOCYANATE, 1-chloro-4-isocyanato-2-(trifluoromethyl)benzene |
| CAS | : 327-78-6 |
| EC number | : 000-000-0 |
| MF | : C ₈ H ₃ ClF ₃ NO |
| MW | : 221.56 |

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

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

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

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_x), Hydrogen chloride gas, Hydrogen fluoride

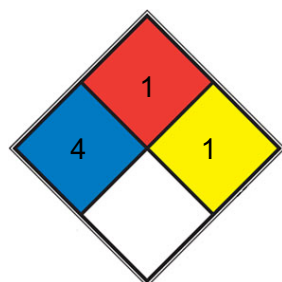
Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

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 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 dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

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 formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Store in cool place. Moisture sensitive.

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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

Safety glasses with side-shields conforming to EN166 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

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government

standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

| | |
|--|--|
| Appearance | white powder |
| Odour | No data available |
| Odour Threshold | No data available |
| pH | No data available |
| Melting point/freezing point | Melting point/range: 40 - 42 °C - lit. |
| Initial boiling point and boiling range | 86 - 90 °C at 19 hPa - lit. |
| Flash point | 99 °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 | No data available |
| 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

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

No data available

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Hydrogen chloride gas, Hydrogen fluoride

Other decomposition products - No data available In the event of fire: see section 5

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 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

Inhalation - May cause respiratory irritation. Inhalation - May cause respiratory irritation. 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.

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

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 2811 IMDG: 2811 IATA: 2811

UN proper shipping name

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (4-Chloro-3-(trifluoromethyl)phenyl isocyanate)

IMDG: TOXIC SOLID, ORGANIC, N.O.S. (4-Chloro-3-(trifluoromethyl)phenyl isocyanate)

IATA: Toxic solid, organic, n.o.s. (4-Chloro-3-(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

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

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

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

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

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

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

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

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

EC Inventory:Not Listed.

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

【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

【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.