

Chemical Safety Data Sheet MSDS / SDS

Isocyanic acid 3,4-dichlorophenyl ester

Revision Date:2025-02-01 Revision Number:1

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

Product identifier

Product name : Isocyanic acid 3,4-dichlorophenyl ester
CBnumber : CB9761511
CAS : 102-36-3
EINECS Number : 203-026-2
Synonyms : 3,4-DICHLOROPHENYL ISOCYANATE, 1,2-dichloro-4-isocyanatobenzene

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

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P405 Store locked up.
P342+P311 IF experiencing respiratory symptoms: call a POISON CENTER or doctor/physician.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P284 Wear respiratory protection.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
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

H317 May cause an allergic skin reaction

H315 Causes skin irritation

H301 Toxic if swallowed

H300 Fatal if swallowed

SECTION 3: Composition/information on ingredients

Substance

Product name	: Isocyanic acid 3,4-dichlorophenyl ester
Synonyms	: 3,4-DICHLOROPHENYL ISOCYANATE, 1,2-dichloro-4-isocyanatobenzene
CAS	: 102-36-3
EC number	: 203-026-2
MF	: C7H3Cl2NO
MW	: 188.01

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. Take victim immediately to hospital. 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 Combustible.

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

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 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

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

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

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

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

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.

Full contact

Material: Nitrile rubber

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

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

Splash contact Material: Nitrile rubber

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

Material tested:Dermatril? (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 CE 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, 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 particle respirator type N99 (US) or type P2 (EN 143) 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.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	beige Solidified mass or fragments
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 41 - 43 °C - lit.
Initial boiling point and boiling range	118 - 120 °C at 24 hPa - lit.
Flash point	123 °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	0,3 hPa at 20 °C 2,0 hPa at 55 °C
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

Heat

Incompatible materials

Water, Alcohols, Strong bases, Amines, acids, Strong oxidizing agents

Hazardous decomposition products

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

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

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 91 mg/kg

LC50 Inhalation - Rat - 4 h - 2.700 mg/m³

Remarks: Sense Organs and Special Senses (Nose, Eye, Ear, and Taste):Eye:Lacrimation. Behavioral:Ataxia. Gastrointestinal:Changes in structure or function of salivary glands.

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: NQ8760000

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Repeated exposure may cause asthma.,
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.

Incompatibilities

Incompatible with oxidizers; contact may cause fires or explosions. Incompatible with amines, aldehydes, alkali metals, ammonia, carboxylic acids, caprolactum, alkaline materials, glycols, ketones, mercaptans, hydrides, organotin catalysts, phenols, strong acids, strong bases, strong reducing agents such as hydrides, urethanes, and ureas.

Waste Disposal

Combustion in an incinerator equipped with afterburner and fume scrubber

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

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UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

IATA:

UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

IATA:

IATA:

UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

Transport hazard class(es)

ADR/RID: - IMDG: - IATA: -

ADR/RID: 2811 IMDG: 2811 IATA: 2811

ADR/RID: - IMDG: - IATA: -

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: 3272 IMDG: 3272 IATA: 3272

ADR/RID: 3272 IMDG: 3272 IATA: 3272

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

ADR/RID: - IMDG: - IATA: -

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: - IMDG: - IATA: -

ADR/RID: - IMDG: - IATA: -

UN proper shipping name

ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

ADR/RID: - IMDG: - IATA: -

ADR/RID: III IMDG: III IATA: III

ADR/RID: - IMDG: - IATA: -

ADR/RID: II IMDG: II IATA: II

ADR/RID: ESTERS, N.O.S. (methyl valerate) IMDG: ESTERS, N.O.S. (methyl valerate) IATA: Esters, n.o.s. (methyl valerate)

ADR/RID: ESTERS, N.O.S. (Ethyl cyclopropanecarboxylate) IMDG: ESTERS, N.O.S. (Ethyl cyclopropanecarboxylate) IATA: Esters, n.o.s. (Ethyl cyclopropanecarboxylate)

ADR/RID: II IMDG: II IATA: II

ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (lloperidone) IMDG: TOXIC SOLID, ORGANIC, N.O.S. (lloperidone) IATA: Toxic solid, organic, n.o.s. (lloperidone)

ADR/RID: - IMDG: - IATA: -

Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

ADR/RID: - IMDG: - IATA: -

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

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: 3 IMDG: 3 IATA: 3

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

ADR/RID: no IMDG Marine pollutant: no IATA: no Special precautions for user Further information Not classified as dangerous in the meaning of transport regulations.

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

ADR/RID: no IMDG Marine pollutant: no IATA: no Special precautions for user Further information Not classified as dangerous in the meaning of transport regulations.

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: - IMDG: - IATA: -

Packaging group

ADR/RID: - IMDG: - IATA: -

ADR/RID: III IMDG: III IATA: III

No data available

No data available

ADR/RID: II IMDG: II IATA: II

ADR/RID: II IMDG: II IATA: II

No data available

ADR/RID: - IMDG: - IATA: -

ADR/RID: III IMDG: III IATA: III

Environmental hazards

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

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

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

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

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

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

Special precautions for user

No data available

No data available

No data available

No data available

No data available

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: Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

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

EC Inventory: Listed.

New Zealand Inventory of Chemicals (NZIoC): Listed. website: <https://www.epa.govt.nz/>

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

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

Vietnam National Chemical Inventory: Not Listed. website: <https://chemicaldata.gov.vn/>

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

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

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.