ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

3-Methoxycarbonyl-4-chlorophenylisothiocyanate

Revision Date:2026-05-31 Revision Number:1

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

Product identifier

Product name	: 3-Methoxycarbonyl-4-chlorophenylisothiocyanate
CBnumber	: CB31114859
CAS	: 91151-68-7

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 Warning

Precautionary statements

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

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P272 Contaminated work clothing should not be allowed out of the workplace.

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P302+P352 IF ON SKIN: wash with plenty of soap and water.

P370+P378 In case of fire: Use … for extinction.

P333+P313 IF SKIN irritation or rash occurs: Get medical advice/attention.

P403+P235 Store in a well-ventilated place. Keep cool.

Hazard statements

H317 May cause an allergic skin reaction

H227 Combustible liquid

SECTION 3: Composition/information on ingredients

Substance

Product name	: 3-Methoxycarbonyl-4-chlorophenylisothiocyanate
CAS	: 91151-68-7
MF	: C9H6ClNO2S
MW	: 227.667

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.Move out of dangerous area.

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 or 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 (NOx), Hydrogen bromide gas

Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

Further information

no data available

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. 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

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.

Normal measures for preventive fire protection.

For precautions see section 2.

Conditions for safe storage, including any incompatibilities

Specific end use(s)

Apart from the uses mentioned in section 1, no other specific uses are stipulated

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SECTION 8: Exposure controls/personal protection

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

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.

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 / Form	no data available
Odor	no data available
Odor Threshold	no data available
pH	no data available
Melting point	no data available
Boiling point/range	no data available
Flash point	no data available
Evapouration rate	no data available
Flammability	no data available
Upper/lower flammability	no data available
explosive limits	no data available
Vapor pressure	no data available
Vapour density	no data available
Relative density	no data available
Water solubility	no data available
Partition coefficient	no data available
Auto-ignition temperature	no data available
Decomposition Temp	no data available

log Pow	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

no data available

Hazardous decomposition products

no data available

Other decomposition products

no data available

In the event of fire

see section 5

SECTION 11: Toxicological information

Acute toxicity

Classified based on available data. For more details, see section 2

Skin corrosion/irritation

Classified based on available data. For more details, see section 2

Serious eye damage/irritation

Classified based on available data. For more details, see section 2

Respiratory or skin sensitisation

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

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.

ACGIH

No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP

No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA

No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

Additional Information

Classified based on available data. For more details, see section 2

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

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

Other adverse effects

no data available

SECTION 13: Disposal considerations

Waste treatment methods

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.

SECTION 14: Transport information

UN number

ADR/RID:

IMDG:

IATA-DGR:

UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

Transport hazard class(es)

ADR/RID:

IMDG:

IATA-DGR:

Packaging group

ADR/RID:

IMDG:

IATA-DGR:

Environmental hazards

ADR/RID: -

IMDG: -

IATA-DGR: -

Special precautions for user

Further information : No data available

SECTION 15: Regulatory information

SARA 302

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

New Jersey Right To Know Components

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox. Acute toxicity

Eye Irrit. Eye irritation

Skin Irrit. Skin irritation

H302 Harmful if swallowed

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

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.