

Chemical Safety Data Sheet MSDS / SDS

5-Methyl-3-phenylisoxazole-4-carboxylic acidRevision Date:2025-06-28 Revision Number:1

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

Product name : 5-Methyl-3-phenylisoxazole-4-carboxylic acid
CBnumber : CB0459352
CAS : 1136-45-4
EINECS Number : 214-497-9
Synonyms : 5-Methyl-3-phenylisoxazole-4-carboxylic acid, OXACILLIN RELATED COMPOUND C

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)

**Precautionary statements**

P330 Rinse mouth.
P270 Do not eat, drink or smoke when using this product.
P264 Wash skin thoroughly after handling.
P264 Wash hands thoroughly after handling.

Hazard statements

H313 May be harmful in contact with skin
H302 Harmful if swallowed

SECTION 3: Composition/information on ingredients**Substance**

Product name	: 5-Methyl-3-phenylisoxazole-4-carboxylic acid
Synonyms	: 5-Methyl-3-phenylisoxazole-4-carboxylic acid, OXACILLIN RELATED COMPOUND C
CAS	: 1136-45-4
EC number	: 214-497-9
MF	: C ₁₁ H ₉ NO ₃
MW	: 203.19

SECTION 4: First aid measures

Description of first aid measures

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration.

In case of skin contact

Wash off with soap and plenty of water.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water.

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)

Advice for firefighters

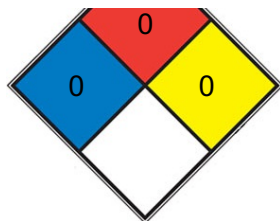
Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704





■ HEALTH	0	Poses no health hazard, no precautions necessary and would offer no hazard beyond that of ordinary combustible materials
■ FIRE	0	Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)
■ 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

Avoid dust formation. Avoid breathing vapours, mist or gas. For personal protection see section 8.

Environmental precautions

No special environmental precautions required.

Methods and materials for containment and cleaning up

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

Provide appropriate exhaust ventilation at places where dust is formed. 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.

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

General industrial hygiene practice.

Personal protective equipment

Eye/face protection

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

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

No special environmental precautions required.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	off-white powder
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 192 - 194 °C
Initial boiling point and boiling range	341.49°C (rough estimate)
Flash point	No data available
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)

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 Intraperitoneal - Rat - 1.500 mg/kg

Remarks: Lungs, Thorax, or Respiration:Dyspnea.

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

No data available

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

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

RTECS: Not available

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.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

SECTION 14: Transport information

UN number

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

IATA:

UN number

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

Transport hazard class(es)

ADR/RID: - IMDG: - IATA: -

ADR/RID: - IMDG: - IATA: -

ADR/RID: 1993 IMDG: 1993 IATA: 1993

ADR/RID: 3077 IMDG: 3077 IATA: 3077

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

ADR/RID: 3077 IMDG: 3077 IATA: 3077

ADR/RID: 2030 IMDG: 2030 IATA: 2030

ADR/RID: - IMDG: - IATA: -

ADR/RID: 1993 IMDG: 1993 IATA: 1993

ADR/RID: 2643 IMDG: 2643 IATA: 2643

ADR/RID: - IMDG: - IATA: -

UN proper shipping name

ADR/RID: METHYL BROMOACETATE IMDG: METHYL BROMOACETATE IATA: Methyl bromoacetate

ADR/RID: FLAMMABLE LIQUID, N.O.S. (3-Chlorobut-1-ene) IMDG: FLAMMABLE LIQUID, N.O.S. (3-Chlorobut-1-ene) IATA: Flammable liquid, n.o.s. (3-Chlorobut-1-ene)

ADR/RID: - IMDG: - IATA: -

ADR/RID: HYDRAZINE, AQUEOUS SOLUTION IMDG: HYDRAZINE, AQUEOUS SOLUTION IATA: Hydrazine, aqueous solution Passenger

Aircraft: Not permitted for transport

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

ADR/RID: II IMDG: II IATA: II

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Methyl 2,5- dichlorobenzoate) IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Methyl 2,5- IATA: Environmentally hazardous substance, solid, n.o.s. dichlorobenzoate)

ADR/RID: FLAMMABLE LIQUID, N.O.S. (2-Isobutylthiazol) IMDG: FLAMMABLE LIQUID, N.O.S. (2-Isobutylthiazol) IATA: Flammable liquid, n.o.s. (2-Isobutylthiazol)

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

ADR/RID: - IMDG: - IATA: -

Environmental hazards

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

ADR/RID: - IMDG: - IATA: -

ADR/RID: 3 IMDG: 3 IATA: 3

(Methyl 2,5- ADR/RID: 9 IMDG: 9 IATA: 9

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

ADR/RID: - IMDG: - IATA: -

ADR/RID: 8 (6.1) IMDG: 8 (6.1) IATA: 8 (6.1)

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

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

Special precautions for user

No data available

ADR/RID: II IMDG: II IATA: II

ADR/RID: II IMDG: II IATA: II

No data available

ADR/RID: II IMDG: II IATA: II

ADR/RID: - IMDG: - IATA: -

No data available

ADR/RID: III IMDG: III IATA: III

ADR/RID: III IMDG: III IATA: III

ADR/RID: - IMDG: - IATA: -

No data available

Environmental hazards

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

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

ADR/RID: yes IMDG Marine pollutant: yes IATA: yes dichlorobenzoate) Special precautions for user Further information EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

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: yes IMDG Marine pollutant: yes 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

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

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

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

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

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:Listed. website: <https://www.epa.gov/>

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

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

EC Inventory: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.