

Carboxine SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- * Product Name: Carboxine
- * Catalog Number: S4805
- * CAS Number: 5234-68-4
- * IUPAC Name: 1,4-Oxathiin-3-carboxamide, 5,6-dihydro-2-methyl-N-phenyl-

Relevant identified uses and uses advised against

- * Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.
- * Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

- * Company: Selleck Chemicals
- * TollFree: +1 877 796-6397
- * Tel: +1 832 582-8158
- * Fax: +1 832 582-8590

Emergency telephone number

- * Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

- Acute toxicity (oral): Category 4. H302
- Skin sensitization: Category 1. H317
- Specific target organ toxicity (repeated exposure): Category 2. H373
- Acute aquatic toxicity: Category 1. H400
- Chronic aquatic toxicity: Category 1. H410

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Warning

Hazard statement(s)

- H302: Harmful if swallowed
- H317: May cause an allergic skin reaction
- H373: May causes damage to organs through prolonged or repeated exposure
- H400: Very toxic to aquatic life
- H410: Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

None.

Prevention	P260: Do not breathe dust/fume/gas/mist/vapors/spray. P261: Avoid breathing dust/fume/gas/mist/vapors/spray. P264: Wash hands thoroughly after handling. P270: Do not eat, drink or smoke when using this product. P272: Contaminated work clothing should not be allowed out of the workplace. P273: Avoid release to the environment. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P301+P317: IF SWALLOWED: Get medical help. P302+P352: IF ON SKIN: wash with plenty of water. P319: Get medical help if you feel unwell. P321: Specific treatment (see information on this label and safety datasheet)). P330: Rinse mouth. P333+P317: If skin irritation or rash occurs: Get medical help. P362+P364: Take off contaminated clothing and wash it before reuse. P391: Collect spillage.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Carboxine

CAS Number: 5234-68-4

PubChem CID: 21307

Molecular formula: C₁₂H₁₃NO₂S

Molecular weight: 235.30 g/mol

IUPAC name: 6-methyl-N-phenyl-2,3-dihydro-1,4-oxathiine-5-carboxamide

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Move to fresh air. Keep at rest in a position comfortable for breathing. Seek medical attention if symptoms persist.

Skin contact: Wash with plenty of soap and water. Remove contaminated clothing. Seek medical attention if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention.

Ingestion: Rinse mouth. Do NOT induce vomiting unless directed by medical personnel. Seek medical attention.

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO₂), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Combustible. Heating may produce toxic fumes.

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

Flash point: 203 °C

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

Carboxin is resistant to mild oxidative and hydrolytic conditions. Alkaline hydrolysis yields the more toxic aniline. If reuse is not possible, incineration appears to be the method of choice for disposal. Recommendable method: Incineration. Not recommendable method: Alkaline hydrolysis.

Avoid contact with skin or clothing. Wash hands and face thoroughly with soap and water after use and before eating or smoking.

SRP: The scientific literature for the use of contact lenses in industry is conflicting. The benefit or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place.

SRP: Local exhaust ventilation should be applied wherever there is an incidence of point source emissions or dispersion of regulated contaminants in the work area. Ventilation control of the contaminant as close to its point of generation is both the most economical and safest method to minimize personnel exposure to airborne contaminants.

SRP: Contaminated protective clothing should be segregated in such a manner so that there is no direct personal contact by personnel who handle, dispose, or clean the clothing. Quality assurance to ascertain the completeness of the cleaning procedures should be implemented before the decontaminated protective clothing is returned for reuse by the workers. Contaminated clothing should not be taken home at end of shift, but should remain at employee's place of work for cleaning.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Store in cool, dry area out of reach of children and animals.

7.2 Conditions for safe storage, including any incompatibilities

Store in cool, dry area out of reach of children and animals.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use in a well-ventilated area. Chemical fume hood recommended for powder handling.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear safety glasses with side shields.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Respiratory protection usually not required under normal use with adequate ventilation.

Use N95 respirator for large-scale powder handling.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- a) Appearance: Carboxin appears as off-white crystals. Systemic fungicide and seed protectant.
- b) Odor: No data available
- c) Odor threshold: No data available
- d) pH: No data available
- e) Melting point/freezing point: 91.5 to 92.5 °C and 98 to 101 °C, reflecting two crystalline structures which revert to one in solution.
- f) Initial boiling point and boiling range: No data available
- g) Flash point: 203 °C
- h) Evaporation rate: No data available
- i) Flammability (solid, gas): No data available
- j) Upper/lower flammability or explosive limits: No data available
- k) Vapor pressure: 0.00000018 [mmHg]
- l) Vapor density: No data available
- m) Relative density: 1.7 g/mL
- n) Water solubility: 221.2 g/L in acetone, 89.33 g/L in methanol, 107.7 g/L in ethyl acetate, all at 20 °C.
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 2.1
- p) Auto-ignition temperature: No data available
- q) Decomposition temperature: No data available
- r) Viscosity: No data available
- s) Explosive properties: No data available
- t) Oxidizing properties: No data available

9.2 Other information

Topological Polar Surface Area (TPSA): 63.6 Å²
Complexity: 295

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.
Avoid strong oxidizing agents, strong acids, and strong bases.

10.5 Incompatible materials

Strong oxidizing agents, strong acids, strong bases.

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Sulfur oxides (SO_x).

See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

No acute toxicity data available.

Skin corrosion/irritation:

No data available.

Serious eye damage/eye irritation:

No data available.

Respiratory or skin sensitization:

May cause an allergic skin reaction (H317).

Germ cell mutagenicity:

No data available.

Carcinogenicity:

No data available.

Reproductive toxicity:

No data available.

Specific target organ toxicity (single exposure):

H373

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information

Carcinogen classification:

No indication of carcinogenicity to humans (not listed by IARC).

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

LD50 *Anas platyrhynchos* (Mallard duck, 14 day old) oral 6094 mg/kg/14 days

LC50 *Anas platyrhynchos* (Mallard duck, 5 day old) dietary >4110 ppm/8 days

LC50 *Colinus virginianus* (Northern bobwhite, juvenile) dietary >1000 ppm/8 days

LC50 *Colinus virginianus* (Northern bobwhite, 5 day old) dietary >5620 ppm/8 days

For more Ecotoxicity Values (Complete) data for CARBOXIN (26 total), please visit the HSDB record page.

/BIRDS and MAMMALS/ Following chronic exposure, mallard ducks (*Anas platyrhynchos*) exhibited reductions in the number of eggs laid, viable embryos, live 3-week embryos, normal hatchlings and 14-day survivors at 700 mg/kg/day.

/AQUATIC SPECIES/ /In/ two freshwater fish toxicity studies... Rainbow trout exposed to the four highest concentration levels (0.93, 1.5, 2.4, and 4.1 mg/L) demonstrated partial to complete loss of equilibrium, lethargy, darkened pigmentation and swimming on the surface. ...Bluegill sunfish exposed to the three highest concentrations, i.e., 2.7, 4.3, and 7.5 mg/L, also demonstrated partial to complete loss of equilibrium, lethargy, darkened pigmentation and swimming on the surface.

6.30e+03

8.20e+04

1.90e+03

5.00e+00

1.00e+00

1.00e-01

Volatile

Mutagen

1

0.1

1.90e+04

2.50e+05

5.70e+03

5.00e+00

1.00e-01

Volatile

Mutagen

1

0.1

Carboxin's production may result in its release to the environment through various waste streams; its use as a fungicide for commercial seed treatment and on-farm seed treatment will result in its direct release to the environment.

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 2.1

Low potential for bioaccumulation (Log P < 3).

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available.

12.6 Other adverse effects

This substance is classified as hazardous to the aquatic environment.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION

14.1 UN number

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: Yes (classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable.

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Not available in public databases.

SARA 302 Components:

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

SARA 313 Components:

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 (short-term) health hazard

Chronic (long-term) health hazard

Environmental hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

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

Other regulatory listings:

- EFSA Legal Basis: Commission Regulation (EC) No 33/2008
- Status Regulation (EC): 2011/52/EU, Reg. (EU) 2022/801, Reg. (EU) No 2018/1266, Reg. (EU) No 2019/324, Reg. (EU) No 540/2011
- Federal Drinking Water Guidelines: EPA 700 ug/L
- FIFRA Requirements: The Agency has completed its assessment of the dietary, occupational, residential, and ecological risk associated with the use of pesticide products containing the active ingredient carboxin. Based on a review of these data and on public comments on the Agency's assessments for the active ingredient

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/09

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product.

Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.