

Dicoumarol SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- * Product Name: Dicoumarol
- * Catalog Number: S4299
- * CAS Number: 66-76-2
- * IUPAC Name: 3,3'-methylenebis[4-hydroxy-2H-1-benzopyran-2-one

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 3. H301
- Acute toxicity (oral): Category 4. H302
- Specific target organ toxicity (single exposure): Category 2. H371
- Specific target organ toxicity (repeated exposure): Category 1. H372
- Specific target organ toxicity (repeated exposure): Category 2. H373
- Chronic aquatic toxicity: Category 2. H411

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)

- H301: Toxic if swallowed
- H302: Harmful if swallowed
- H371: May cause damage to organs
- H372: Causes damage to organs through prolonged or repeated exposure
- H373: May causes damage to organs through prolonged or repeated exposure
- H411: Toxic to aquatic life with long lasting effects

Precautionary statement(s)

None.

Prevention	P260: Do not breathe dust/fume/gas/mist/vapors/spray. P264: Wash hands thoroughly after handling. P270: Do not eat, drink or smoke when using this product. P273: Avoid release to the environment.
Response	P301+P316: IF SWALLOWED: Get emergency medical help immediately. P301+P317: IF SWALLOWED: Get medical help. P308+P316: IF exposed or concerned: Get emergency medical help immediately. P319: Get medical help if you feel unwell. P321: Specific treatment (see information on this label and safety datasheet)). P330: Rinse mouth. P391: Collect spillage.
Storage	P405: Store locked up.
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: Dicoumarol

CAS Number: 66-76-2

PubChem CID: 54676038

Molecular formula: C₁₉H₁₂O₆

Molecular weight: 336.3 g/mol

IUPAC name: 4-hydroxy-3-[(4-hydroxy-2-oxochromen-3-yl)methyl]chromen-2-one

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.

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.

WARNING: Highly toxic — only trained personnel should handle spills.

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: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

Care should be taken ... not to contaminate foodstuffs ... not to leave material within reach of children; to use prepared baits rather than scatter poison; to collect and destroy dead rodents; to bury baits and powder when operation is completed. /coumarin derivatives/

Wherever possible, toxic chemicals, concentrates & bait preparations should be handled in a fume cupboard. When bait mixing has been done in the field, operators should take care to remain sheltered from the wind.

/Rodenticides/

Scrupulous personal hygiene must be adhered to when dealing with poisons. All cuts & abrasions on the hands & forearms must be covered with waterproof adhesive dressings before any operations are started. When the work is finished or when a break is taken in the middle /of the day/, protective clothing should be removed & hands washed thoroughly with soap & hot water. Contaminated protective clothing must not be taken into "clean" areas.

/Rodenticides/

Smoking, eating & drinking must be strictly prohibited in all rooms in which poisons are present. /Rodenticides/

For more Preventive Measures (Complete) data for DICUMAROL (7 total), please visit the HSDB record page.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Dicumarol should be stored in well-closed containers at a temperature below 40 degrees C (104 °F), preferably 15 to 30 °C (59 to 86 °F), and kept away from direct sunlight. The manufacturer recommends storage below 25 °C (77 °F).

7.2 Conditions for safe storage, including any incompatibilities

Dicumarol should be stored in well-closed containers at a temperature below 40 degrees C (104 °F), preferably 15 to 30 °C (59 to 86 °F), and kept away from direct sunlight. The manufacturer recommends storage below 25 °C (77 °F).

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: White solid with a mild pleasant odor; [HSDB]

b) Odor: Slight, pleasant odor

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: 287-293 °C

f) Initial boiling point and boiling range: No data available

- g) Flash point: No data available
- 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: No data available
- l) Vapor density: No data available
- m) Relative density: No data available
- n) Water solubility: Practically insol in water, alc, ether.
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 2.6
- 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): 93.1 Å²

Complexity: 605

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.

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).

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:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

No data available.

Reproductive toxicity:

No data available.

Specific target organ toxicity (single exposure):

H371, H372, 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).

Exposure routes:

Oral, dermal, inhalation, and parenteral (contaminated drugs). (A3101)

Signs and symptoms of exposure:

Dicoumarol can cause bleeding complications. (L1960)

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

LC50 Pimephales promelas (fathead minnow) 5.11 mg/l/96 hr (95% confidence limit 4.18 - 6.24 mg/l), flow-through bioassay with measured concentrations, 24.5 °C, dissolved oxygen 7.2 mg/l, hardness 44.3 mg/l calcium carbonate, alkalinity 44.0 mg/l calcium carbonate, and pH 7.8.

Dicoumarol's production and use in anticoagulant therapy may result in its release to the environment through various waste streams; its former use as a rodenticide resulted in its direct release to the environment. The compound has been isolated from spoiled sweet clover hay. If released to air, an estimated vapor pressure of 6.0×10^{-17} mm Hg at 25 °C indicates dicoumarol will exist solely in the particulate phase in the ambient atmosphere. Particulate-phase dicoumarol will be removed from the atmosphere by wet and dry deposition. If released to soil, dicoumarol is expected to have moderate mobility based upon an estimated Koc of 320. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 1.4×10^{-13} atm-cu m/mole. If released into water, dicoumarol is expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. An estimated BCF of 8 suggests the potential for bioconcentration in aquatic organisms is low. Occupational exposure to dicoumarol may occur through inhalation and

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 2.6

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**

UN 3027

14.2 UN proper shipping name

Coumarin derivative pesticides, solid, toxic, NOS

14.3 Transport hazard class(es)

Consult official transport regulations (DOT/IATA/IMDG) for hazard classification.

14.4 Packing group

Consult official transport regulations (DOT/IATA/IMDG) for packing group assignment.

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:

- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Developmental Toxicity Authoritative List - Prop 65 Report - regardless of intended function of ingredient in the product
- FDA Requirements: The Approved Drug Products with Therapeutic Equivalence Evaluations List identifies discontinued drug products. Dicumarol is included on this list.

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.