Coumarin SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Coumarin
* Catalog Number: S4170
* CAS Number: 91-64-5
* IUPAC Name: 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

Skin sensitization: Category 1. H317

Specific target organ toxicity (repeated exposure): Category 2. H373

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 H317: May cause an allergic skin reaction H373: May causes damage to organs through prolonged or repeated exposure
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. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P301+P316: IF SWALLOWED: Get emergency medical help immediately. 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.
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: Coumarin

CAS Number: 91-64-5

PubChem CID: 323

Molecular formula: C9H6O2

Molecular weight: 146.14 g/mol

IUPAC name: chromen-2-one

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Fresh air, rest.

Skin contact: Remove contaminated clothes. Rinse and then wash skin with water and soap.

Eye contact: First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Ingestion: Rinse mouth. Refer for 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 (CO_2), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. A water spray may also be used. (NTP, 1992)

Use water spray, foam, powder, carbon dioxide.

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: 304 °F (NTP, 1992)

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

Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.

FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Carefully collect remainder. Then store and dispose of according to local regulations.

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.

Incineration: Coumarin should be combined with paper or other flammable material. An alternate procedure is to dissolve the solid in a flammable solvent and spray the soln into the fire chamber.

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.

...Substitution of less irritating substances, ...redesign of operations...prevent contact, provision of a physical barrier against contact, proper washing facilities, work clothing and storage facilities, protective clothing, and barrier creams. Medical control... .

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

SMALL SPILLS AND LEAKAGE: Should a spill occur while you are handling this chemical, FIRST REMOVE ALL SOURCES OF IGNITION, then you should dampen the solid spill material with 60-70% ethanol and transfer the dampened material to a suitable container. Use absorbent paper dampened with 60-70% ethanol to pick up any remaining material. Seal the absorbent paper, and any of your clothes, which may be contaminated, in a vapor-tight plastic bag for eventual disposal. Solvent wash all contaminated surfaces with 60-70% ethanol followed by washing with a soap and water solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned.

STORAGE PRECAUTIONS: You should protect this material from exposure to light. Keep it away from oxidizing materials and store it under refrigerated temperatures. (NTP, 1992)

Separated from food and feedstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Separated from food and feedstuffs.

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: Coumarin appears as colorless crystals, flakes or colorless to white powder with a pleasant fragrant vanilla odor and a bitter aromatic burning taste. (NTP, 1992)

b) Odor: Pleasant, fragrant odor resembling that of vanilla beans.

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: 154 to 158 °F (NTP, 1992)

f) Initial boiling point and boiling range: 568 °F at 760 mmHg (NTP, 1992)

g) Flash point: 304 °F (NTP, 1992)

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: 0.01 mmHg at 117 °F ; 1 mmHg at 223 °F (NTP, 1992)

l) Vapor density: No data available

m) Relative density: 0.935 at 68 °F (NTP, 1992) - Less dense than water; will float

n) Water solubility: less than 0.1 mg/mL at 63.5 °F (NTP, 1992)

o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 1.4

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): 26.3 Å²

Complexity: 196

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 (CO□).

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:

Coumarin

Group 3: Not classifiable as to its carcinogenicity to humans

Volume Sup 7: Overall Evaluations of Carcinogenicity: An Updating of IARC Monographs Volumes 1 to 42, 1987; 440 pages; ISBN 92-832-1411-0 (out of print)

Volume 77: (2000) Some Industrial Chemicals

2000

2000

Coumarin

TR-422: Toxicology and Carcinogenesis Studies of Coumarin (CASRN 91-64-5) in F344/N Rats and B6C3F1 Mice (Gavage Studies) (1993)

06/23/92

Some Evidence

Equivocal Evidence

Some Evidence

Clear Evidence

Under the

Exposure routes:

The substance can be absorbed into the body by inhalation of its aerosol, through the skin and by ingestion.

Signs and symptoms of exposure:

MAY BE ABSORBED! Redness. Pain.

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

/ACCIDENTAL POISONINGS/ Coumarin, contained in sweetclover hay (melilotus spp), is converted to dicoumarin by molds under certain conditions. This compound interferes with prothrombin synthesis and results in hemorrhagic disease when molded sweetclover hay is ingested over period of time.

Coumarin's production and use as a fragrance ingredient in soaps, detergents, lotions, perfumes, tobacco, household products and as a pharmaceutical flavoring may result in its release to the environment through various waste streams. Coumarin is a naturally occurring compound found in a large number of plants belonging to many different families, including lavender oil, woodruff (Asperula species), and sweet clover (Melilotus). If released to air, a vapor pressure of 9.8X10-4 mm Hg at 25 °C indicates coumarin will exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase coumarin will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 29 hrs. Particulate-phase coumarin will be removed from the atmosphere by wet and dry deposition. Direct photlyisis may be an important environmental fate process based on a 59.2% mineralization to CO2 when exposed to UV radiation >290 nm for 17 hr. If released to soil, coumarin is expected to have high mobility based upon an estimated Koc of 140. Biodegradation in soil may be an important environmental fate process based on 100% degrad

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 1.4

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

No other adverse ecological effects identified.

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)

Class 6.1

DOT label: Poison

14.4 Packing group

Packing group I, II, III

14.5 Environmental hazards

Marine pollutant: No (not 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: Registered (REACH Active)

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

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:

- The Australian Inventory of Industrial Chemicals: Chemical: 2H-1-Benzopyran-2-one

- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Fragrance Allergen Authoritative List - Annex III of the EU Cosmetics Regulation No. 1223/2009 - Fragrance Allergens Report - if present in a rinse-off cosmetic product at a concentrat

- EFSA Legal Basis: Regulation (EC) No 178/2002 (amended)

- FDA Requirements: (a) Coumarin is the chemical 1,2-benzopyrone, C9H6O2. It is found in tonka beans and extract of tonka beans, among other natural sources, and is also synthesized. It has been used as a flavoring agent. (b) Food containing any added coumarin as such or as a constituent of tonka beans or tonka extract

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.