

## SAFETY DATA SHEET

Version 6.8  
Revision Date 09/08/2024  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Coumarin

Product Number : C4261  
Brand : Sigma  
CAS-No. : 91-64-5

**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Acute toxicity, Oral (Category 3), H301  
Acute toxicity, Dermal (Category 3), H311  
Skin sensitization (Category 1), H317

For the full text of the H-Statements mentioned in this Section, see Section 16.

Sigma - C4261

Page 1 of 11

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H301 + H311

Toxic if swallowed or in contact with skin.

H317

May cause an allergic skin reaction.

Precautionary Statements

P261

Avoid breathing dust.

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P272

Contaminated work clothing must not be allowed out of the workplace.

P280

Wear protective gloves/ protective clothing.

P301 + P310 + P330

IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.

P302 + P352 + P312

IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.

P333 + P313

If skin irritation or rash occurs: Get medical advice/ attention.

P362

Take off contaminated clothing and wash before reuse.

P405

Store locked up.

P501

Dispose of contents/ container to an approved waste disposal plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Synonyms : 1,2-Benzopyrone  
1-Benzopyran-2-one  
2H-Chromen-2-one

Formula : C<sub>9</sub>H<sub>6</sub>O<sub>2</sub>

Molecular weight : 146.14 g/mol

CAS-No. : 91-64-5

EC-No. : 202-086-7

| Component                    | Classification                               | Concentration |
|------------------------------|--|---------------|
| <b>2H-1-benzopyran-2-one</b> |  |               |
|                              | Acute Tox. 3; Skin Sens. 1; H301, H311, H317 | <= 100 %      |

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

#### If swallowed

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

### 4.2 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

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### 5.4 Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Avoid generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.  
For personal protection see section 8.

### **6.2 Environmental precautions**

Do not let product enter drains.

### **6.3 Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

For precautions see section 2.2.

### **7.2 Conditions for safe storage, including any incompatibilities**

#### **Storage conditions**

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

#### **Storage class**

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

### **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.

### **8.2 Exposure controls**

#### **Appropriate engineering controls**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

## 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). Safety glasses

### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

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Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

### Body Protection

protective clothing

### Respiratory protection

Recommended Filter type: Filter type P3

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.  
required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

### Control of environmental exposure

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |               |                                  |
|---------------|----------------------------------|
| a) Appearance | Form: flakes<br>Color: colorless |
| b) Odor       | pleasant                         |

|   |  |
|---|--|
| c) Odor Threshold                               | No data available                                      |
| d) pH   | No data available                                      |
| e) Melting point/freezing point                 | Melting point/ range: 68 - 73 °C (154 - 163 °F) - lit. |
| f) Initial boiling point and boiling range      | 298 °C 568 °F - lit.                                   |
| g) Flash point                                  | 162 °C (324 °F) - closed cup                           |
| 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) Density                                      | ca.0.935 kg/m <sup>3</sup> at 20 °C (68 °F)            |
| Relative density                                | ca.0.93520 °C - OPPTS 830.7300                         |
| n) Water solubility                             | ca.1.9 g/l at 20 °C (68 °F) - US-EPA                   |
| o) Partition coefficient: n-octanol/water       | No data available                                      |
| p) Autoignition temperature                     | No data available                                      |
| q) Decomposition temperature                    | No data available                                      |
| r) Viscosity                                    | No data available                                      |
| s) Explosive properties                         | No data available                                      |
| t) Oxidizing properties                         | none   |

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Sigma - C4261

Page 6 of 11

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:  
Strong oxidizing agents  
Strong acids  
strong alkalis

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

no information available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - 293 mg/kg

Remarks: (ECHA)

Inhalation: No data available

LD50 Dermal - Rat - 293 mg/kg

Remarks: (ECHA)

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(Regulation (EC) No. 440/2008, Annex, B.4)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 4 Days

(US-EPA)

#### Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: positive

(OECD Test Guideline 429)

#### Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: positive

Test Type: In vitro mammalian cell gene mutation test  
Test system: Chinese hamster ovary cells  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 476  
Result: negative

Test Type: In vivo micronucleus test  
Species: Mouse  
Cell type: Bone marrow  
Application Route: Oral  
Method: OECD Test Guideline 474  
Result: negative

### **Carcinogenicity**

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient 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 on OSHA's list of regulated carcinogens.

### **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

## **11.2 Additional Information**

Repeated dose toxicity - Mouse - male and female - Oral - 13 Weeks - NOAEL (No observed adverse effect level) - > 138.3 mg/kg

Remarks: (ECHA)

RTECS: GN4200000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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Systemic effects:

If swallowed

Possible symptoms:

depressed respiration



Drowsiness  
narcosis

Toxic effect on:

Liver  
Kidney

Substances which occur in nature

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

Toxicity to daphnia and other aquatic invertebrates      Remarks: No data available  
(2H-1-benzopyran-2-one)

Toxicity to bacteria

### **12.2 Persistence and degradability**

Biodegradability      aerobic - Exposure time 28 d  
Result: ca.90 % - Readily biodegradable.  
(OECD Test Guideline 301F)

### **12.3 Bioaccumulative potential**

No data available

### **12.4 Mobility in soil**

No data available

### **12.5 Results of PBT and vPvB assessment**

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

### **12.6 Endocrine disrupting properties**

No data available

### **12.7 Other adverse effects**

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14: Transport information

#### DOT (US)

UN number: 2811    Class: 6.1    Packing group: III  
Proper shipping name: Toxic solids, organic, n.o.s. (2H-1-benzopyran-2-one)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

UN number: 2811    Class: 6.1    Packing group: III    EMS-No: F-A, S-A  
Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (2H-1-benzopyran-2-one)

#### IATA

UN number: 2811    Class: 6.1    Packing group: III  
Proper shipping name: Toxic solid, organic, n.o.s. (2H-1-benzopyran-2-one)

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## SECTION 15: Regulatory information

#### CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

#### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

#### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Acute Health Hazard  
Chronic Health Hazard

**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.

#### US State Regulations

##### Massachusetts Right To Know

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

##### Maine Chemicals of High Concern

Sigma - C4261

Page 10 of 11

Product does not contain any listed chemicals

**Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

**Washington Chemicals of High Concern**

Product does not contain any listed chemicals

**The ingredients of this product are reported in the following inventories:**

TSCA : All substances listed as active on the TSCA inventory

**TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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**SECTION 16: Other information**

**Further information**

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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