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

1.1 Product identifiers

Product name: Coumarin
Product Number: W526509
Brand: Aldrich
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

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.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal Word: Danger

Aldrich - W526509
Hazard statement(s)
H301 + H311  Toxic if swallowed or in contact with skin.
H317    May cause an allergic skin reaction.

Precautionary statement(s)
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: Coumarin, Chinese
1,2-Benzopyrone
1-Benzopyran-2-one

Formula: C₉H₆O₂
Molecular weight: 146.14 g/mol
CAS-No.: 91-64-5
EC-No.: 202-086-7

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>2H-1-benzopyran-2-one</td>
<td>Acute Tox. 3; Skin Sens. 1; H301, H311, H317</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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

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

SECTION 5: Firefighting measures

5.1 Extinguishing media
Suitable extinguishing media
- Water
- Foam
- Carbon dioxide (CO2)
- 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.

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.
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.

**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

**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).

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

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).

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.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- **Appearance**
  - Form: flakes
  - Color: colorless

- **Odor**
  - pleasant

- **Odor Threshold**
  - No data available

- **pH**
  - No data available

- **Melting point/freezing point**
  - Melting point/range: 68 - 73 °C (154 - 163 °F) - lit.

- **Initial boiling point and boiling range**
  - 298 °C 568 °F - lit.

- **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/m³ 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

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).

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

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

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.

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

SECTION 12: Ecological information

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

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

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.
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
Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (2H-1-benzopyran-2-one)
EMS-No: F-A, S-A

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

SECTION 15: Regulatory information

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

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 Health Hazard, Chronic Health Hazard

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

SECTION 16: Other information

Further information
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada