

## SAFETY DATA SHEET

Version 6.1  
Revision Date 02/25/2021  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2-Coumaranone

Product Number : 124591  
Brand : Aldrich  
CAS-No. : 553-86-6

**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)**

Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
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 : Warning

Hazard statement(s)  
H315 : Causes skin irritation.

|                            |                                                                                                                                  |
|----------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| H317                       | May cause an allergic skin reaction.                                                                                             |
| H319                       | Causes serious eye irritation.                                                                                                   |
| Precautionary statement(s) |                                                                                                                                  |
| P261                       | Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.                                                                            |
| P264                       | Wash skin thoroughly after handling.                                                                                             |
| P272                       | Contaminated work clothing must not be allowed out of the workplace.                                                             |
| P280                       | Wear protective gloves/ eye protection/ face protection.                                                                         |
| P302 + P352                | IF ON SKIN: Wash with plenty of soap and water.                                                                                  |
| P305 + P351 + P338         | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P333 + P313                | If skin irritation or rash occurs: Get medical advice/ attention.                                                                |
| P337 + P313                | If eye irritation persists: Get medical advice/ attention.                                                                       |
| P362                       | Take off contaminated clothing and wash before reuse.                                                                            |
| 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

|                  |                                                |
|------------------|------------------------------------------------|
| Formula          | : C <sub>8</sub> H <sub>6</sub> O <sub>2</sub> |
| Molecular weight | : 134.13 g/mol                                 |
| CAS-No.          | : 553-86-6                                     |
| EC-No.           | : 209-052-0                                    |

| Component                    | Classification                                                     | Concentration |
|------------------------------|--------------------------------------------------------------------|---------------|
| <b>(3H)-Benzofuran-2-one</b> |                                                                    |               |
|                              | Skin Irrit. 2; Eye Irrit. 2A;<br>Skin Sens. 1; H315, H319,<br>H317 | <= 100 %      |

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

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**If swallowed**

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

**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**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

Carbon oxides

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

No data available

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust.  
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**

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

**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****Advice on safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.**Advice on safe handling**

Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

#### **Advice on protection against fire and explosion**

Provide appropriate exhaust ventilation at places where dust is formed.

#### **Hygiene measures**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

For precautions see section 2.2.

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

#### **Storage conditions**

Keep container tightly closed in a dry and well-ventilated place.

Storage class (TRGS 510): 11: Combustible Solids

### **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**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### **Personal protective equipment**

##### **Eye/face protection**

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

##### **Skin protection**

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

##### **Body Protection**

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### **Respiratory protection**

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### **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: solid<br>Color: light orange                    |
| b) Odor                                         | aromatic                                              |
| c) Odor Threshold                               | No data available                                     |
| d) pH                                           | No data available                                     |
| e) Melting point/freezing point                 | Melting point/range: 49 - 51 °C (120 - 124 °F) - lit. |
| f) Initial boiling point and boiling range      | 248 - 250 °C 478 - 482 °F - lit.                      |
| g) Flash point                                  | 125 °C (257 °F) - ISO 3679                            |
| 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                               | 0.027 hPa at 10 °C (50 °F) - OECD Test Guideline 104  |
| l) Vapor density                                | No data available                                     |
| m) Relative density                             | 1.19 at 50 °C (122 °F)                                |
| n) Water solubility                             | 3.8 g/l at 30 °C (86 °F)                              |
| o) Partition coefficient: n-octanol/water       | log Pow: 1.347 -                                      |
| 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                         | No data available                                     |

### 9.2 Other safety information

|                 |                            |
|-----------------|----------------------------|
| Surface tension | 63.8 mN/m at 20 °C (68 °F) |
|-----------------|----------------------------|

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### **10.3 Possibility of hazardous reactions**

No data available

### **10.4 Conditions to avoid**

No data available

### **10.5 Incompatible materials**

Strong oxidizing agents

### **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 - > 2,000 mg/kg

(OECD Test Guideline 401)

Inhalation: No data available

Dermal: No data available

No data available

#### **Skin corrosion/irritation**

Skin - Rabbit

Result: Irritating to skin.

(OECD Test Guideline 404)

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Irritating to eyes.

(OECD Test Guideline 405)

#### **Respiratory or skin sensitization**

- Mouse

Result: May cause sensitization by skin contact.

#### **Germ cell mutagenicity**

Ames test

S. typhimurium

Result: negative

#### **Carcinogenicity**

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

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**

Not available

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

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**SECTION 12: Ecological information****12.1 Toxicity**

|                                                     |                                                                                                                 |
|-----------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|
| Toxicity to fish                                    | semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - 6.09 mg/l - 96 h<br>(OECD Test Guideline 203)     |
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - Daphnia magna (Water flea) - > 100 mg/l - 48 h<br>(OECD Test Guideline 202)                  |
| Toxicity to algae                                   | static test EC50 - Pseudokirchneriella subcapitata (green algae) - 1.8 mg/l - 72 h<br>(OECD Test Guideline 201) |

**12.2 Persistence and degradability**

|                  |                                                                                                     |
|------------------|-----------------------------------------------------------------------------------------------------|
| Biodegradability | aerobic - Exposure time 28 d<br>Result: 89 % - Readily biodegradable.<br>(OECD Test Guideline 301B) |
|------------------|-----------------------------------------------------------------------------------------------------|

**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 Other adverse effects**

No data available

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**SECTION 13: Disposal considerations****13.1 Waste treatment methods****Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**  
Dispose of as unused product.

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## SECTION 14: Transport information

### **DOT (US)**

Not dangerous goods

### **IMDG**

Not dangerous goods

### **IATA**

Not dangerous goods

### **Further information**

Not classified as dangerous in the meaning of transport regulations.

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## SECTION 15: Regulatory information

### **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 Health Hazard

### **Massachusetts Right To Know Components**

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

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

### **Pennsylvania Right To Know Components**

|                       |                     |               |
|-----------------------|---------------------|---------------|
| (3H)-Benzofuran-2-one | CAS-No.<br>553-86-6 | Revision Date |
|-----------------------|---------------------|---------------|

|                       |                     |               |
|-----------------------|---------------------|---------------|
| (3H)-Benzofuran-2-one | CAS-No.<br>553-86-6 | Revision Date |
|-----------------------|---------------------|---------------|

### **New Jersey Right To Know Components**

|                       |                     |               |
|-----------------------|---------------------|---------------|
| (3H)-Benzofuran-2-one | CAS-No.<br>553-86-6 | Revision Date |
|-----------------------|---------------------|---------------|

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## SECTION 16: Other information

### Further information

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