

SAFETY DATA SHEET

Version 6.3
Revision Date 04/01/2022
Print Date 06/01/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : 3-(α -Acetonylbenzyl)-4-hydroxycoumarin sodium salt

Product Number : A4571
Brand : Aldrich
CAS-No. : 129-06-6

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)**

Acute toxicity, Oral (Category 2), H300
Reproductive toxicity (Category 1B), H360
Short-term (acute) aquatic hazard (Category 3), H402
Long-term (chronic) aquatic hazard (Category 3), H412

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

Hazard statement(s)	
H300	Fatal if swallowed.
H360	May damage fertility or the unborn child.
H412	Harmful to aquatic life with long lasting effects.
Precautionary statement(s)	
P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
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	: 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin
Formula	: C ₁₉ H ₁₅ NaO ₄
Molecular weight	: 330.31 g/mol
CAS-No.	: 129-06-6
EC-No.	: 204-929-4

Component	Classification	Concentration
Warfarin sodium		
	Acute Tox. 2; Repr. 1B; Aquatic Acute 3; Aquatic Chronic 3; H300, H360, H402, H412	<= 100 %
2-Propanol		
	Flam. Liq. 2; Eye Irrit. 2A; STOT SE 3; H225, H319, H336 Concentration limits: >= 20 %: STOT SE 3, H336;	>= 1 - < 5 %

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

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. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. 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

Sodium oxides

Combustible.

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

Suppress (knock down) gases/vapors/mists with a water spray jet. 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 inhalation of dusts. 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.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture.

Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

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): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

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

Component	CAS-No.	Value	Control parameters	Basis
2-Propanol	67-63-0	TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen		

		STEL	400 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Not classifiable as a human carcinogen		
		ST	500 ppm 1,225 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	400 ppm 980 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	400 ppm 980 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		STEL	500 ppm 1,225 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	400 ppm 980 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		PEL	400 ppm 980 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	500 ppm 1,225 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
2-Propanol	67-63-0	Acetone	40 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift at end of workweek			

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands 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

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.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

protective clothing

Respiratory protection

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

- | | |
|---|--|
| a) Appearance | Form: crystalline
Color: colorless |
| b) Odor | odorless |
| c) Odor Threshold | No data available |
| d) pH | 7.2 - 8.3 at ca.1 g/l at 20 °C (68 °F) |
| e) Melting point/freezing point | Melting point/range: 161 °C (322 °F) |
| 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 | 1 hPa at 106 °C (223 °F) |
| l) Vapor density | No data available |
| m) Density | No data available |

Aldrich - A4571

Page 6 of 10

	Relative density	No data available
n)	Water solubility	insoluble
o)	Partition coefficient: n-octanol/water	log Pow: 2.52 at 20 °C (68 °F)
p)	Autoignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	Not classified as explosive.
t)	Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

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

Reacts with air to form peroxides.

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

Strong bases, Acid chlorides, Acid anhydrides

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

Acute toxicity estimate Oral - 9.06 mg/kg

(Calculation method)

LD50 Oral - Rat - 8.7 mg/kg (Warfarin sodium)

Remarks: Blood: Hemorrhage.

(RTECS)

Acute toxicity estimate Inhalation - 4 h - > 200 mg/l - vapor (Calculation method)

Dermal: No data available

Aldrich - A4571

Page 7 of 10

No 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

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

May cause congenital malformation in the fetus. (Warfarin sodium)

Presumed human reproductive toxicant (Warfarin sodium)

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

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

Warfarin suppresses the formation in the liver of prothrombin and factors VII, IX and X resulting in reduced blood clotting capabilities, increased capillary fragility and significant risk of hemorrhage. Warfarin is a cumulative poison, although acute poisonings have occurred from significantly large single doses. Manifestations of poisoning may be delayed for a few days to weeks. Signs of poisoning include nose bleeds, bleeding gums, pallor, hematomas around joints and buttocks, and blood in the urine and feces. Other symptoms include back pain, bleeding lips, mucous membrane hemorrhage, abdominal pain, gastrointestinal bleeding, vomiting, and petechial rash. Dermatological effects have included skin necrosis and alopecia. Later effects of warfarin poisoning may include paralysis due to cerebral hemorrhage and finally hemorrhagic shock and death. There are no immediate warning signs of warfarin overexposure., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (Warfarin sodium)

Stomach - Irregularities - Based on Human Evidence

Kidney - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence
(Warfarin sodium)

SECTION 12: Ecological information

12.1 Toxicity

No data available

12.2 Persistence and degradability

No data available

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 1544 Class: 6.1 Packing group: II
Proper shipping name: Alkaloid salts, solid, n.o.s. (Warfarin sodium)
Reportable Quantity (RQ): 104 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 1544 Class: 6.1 Packing group: II EMS-No: F-A, S-A
Proper shipping name: ALKALOIDS SALTS, SOLID, N.O.S. (Warfarin sodium)

IATA

UN number: 1544 Class: 6.1 Packing group: II
Proper shipping name: Alkaloid salts, solid, n.o.s. (Warfarin sodium)

SECTION 15: Regulatory information

SARA 302 Components

Warfarin sodium

CAS-No.
129-06-6Revision Date
2008-11-03**SARA 313 Components**

The following components are subject to reporting levels established by SARA Title III, Section 313:

Warfarin sodium

CAS-No.
129-06-6Revision Date
2008-11-03

2-Propanol

67-63-0

2007-03-01

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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Version: 6.3

Revision Date: 04/01/2022

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