

SAFETY DATA SHEET

Version 3.10
Revision Date 11/05/2014
Print Date 11/24/2014

1. PRODUCT AND COMPANY IDENTIFICATION**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, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

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
Acute aquatic toxicity (Category 3), H402
Chronic aquatic toxicity (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
H360
H412

Fatal if swallowed.
May damage fertility or the unborn child.
Harmful to aquatic life with long lasting effects.

Precautionary statement(s)

P201
P202

Obtain special instructions before use.
Do not handle until all safety precautions have been read and understood.

P264
P270
P273

Wash skin thoroughly after handling.
Do not eat, drink or smoke when using this product.
Avoid release to the environment.

P281 Use personal protective equipment as required.
P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. 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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin
Formula : C₁₉H₁₅NaO₄
Molecular weight : 330.31 g/mol
CAS-No. : 129-06-6

Hazardous components

Component	Classification	Concentration
Warfarin sodium		
	Acute Tox. 2; Repr. 1B; Aquatic Acute 3; Aquatic Chronic 3; H300, H360, H412	<= 100 %
2-Propanol		
	Flam. Liq. 2; Eye Irrit. 2A; STOT SE 3; H225, H319, H336	>= 5 - < 10 %

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this 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. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

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

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, Sodium oxides

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.
For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. 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.

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

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

Storage class (TRGS 510): Non-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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components 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	Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Not classifiable as a human carcinogen		
		STEL	400 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation Substances for which there is a Biological Exposure Index or Indices (see BEI® section)		

		Not classifiable as a human carcinogen		
		TWA	400 ppm 980 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		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. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	400 ppm 980 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	500 ppm 1,225 mg/m3	USA. NIOSH Recommended Exposure Limits

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
2-Propanol	67-63-0	Acetone	40.0000 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift at end of workweek			

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

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.

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:Dermatril® (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 CE 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

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

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the

sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: crystalline
Colour: colourless |
| b) Odour | odourless |
| c) Odour 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) Vapour pressure | 1 hPa (1 mmHg) at 106 °C (223 °F) |
| l) Vapour density | No data available |
| m) 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) 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 safety information

No data available

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 bases, Acid chlorides, Acid anhydrides

10.6 Hazardous decomposition products

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Inhalation: No data available

Inhalation: No data available (Warfarin sodium)

Dermal: No data available

Dermal: No data available (Warfarin sodium)

No data available

No data available (Warfarin sodium)

Skin corrosion/irritation

No data available

No data available (Warfarin sodium)

Serious eye damage/eye irritation

No data available

No data available (Warfarin sodium)

Respiratory or skin sensitisation

No data available

No data available (Warfarin sodium)

Germ cell mutagenicity

No data available

No data available (Warfarin sodium)

Carcinogenicity

IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (2-Propanol)

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

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

Presumed human reproductive toxicant (Warfarin sodium)

No data available

No data available (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

Additional Information

RTECS: Not available

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)

Kidney - Irregularities - Based on Human Evidence (2-Propanol)

12. ECOLOGICAL INFORMATION

12.1 Toxicity

No data available

Toxicity to fish LC50 - Oncorhynchus mykiss (rainbow trout) - > 16 mg/l - 96 h (Warfarin sodium)

Toxicity to daphnia and EC50 - Daphnia magna (Water flea) - > 17 mg/l - 48 h (Warfarin sodium)
other aquatic
invertebrates

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 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Harmful to aquatic life.

No data available

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. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

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: ALKALOID 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)

15. REGULATORY INFORMATION

SARA 302 Components

The following components are subject to reporting levels established by SARA Title III, Section 302:

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

SARA 313 Components

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

	CAS-No.	Revision Date
2-Propanol	67-63-0	1987-01-01
Warfarin sodium	129-06-6	2008-11-03

SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Warfarin sodium	129-06-6	2008-11-03
2-Propanol	67-63-0	1987-01-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Warfarin sodium	129-06-6	2008-11-03
2-Propanol	67-63-0	1987-01-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Warfarin sodium	129-06-6	2008-11-03
2-Propanol	67-63-0	1987-01-01

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H300	Fatal if swallowed.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.
H360	May damage fertility or the unborn child.
H402	Harmful to aquatic life.

H412 Harmful to aquatic life with long lasting effects.
Repr. Reproductive toxicity
STOT SE Specific target organ toxicity - single exposure

HMIS Rating

Health hazard: 4
Chronic Health Hazard: *
Flammability: 0
Physical Hazard 0

NFPA Rating

Health hazard: 3
Fire Hazard: 0
Reactivity Hazard: 0

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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