

SAFETY DATA SHEET

Creation Date 13-Sep-2013

Revision Date 28-Dec-2021

Revision Number 7

1. Identification

Product Name 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin

Cat No. : AC454680000; AC454680100

CAS No 81-81-2
Synonyms Coumafene ; Warfarin

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute oral toxicity	Category 1
Acute dermal toxicity	Category 1
Acute Inhalation Toxicity - Dusts and Mists	Category 1
Reproductive Toxicity	Category 1A
Specific target organ toxicity - (repeated exposure)	Category 1
Target Organs - Blood.	

Label Elements

Signal Word
Danger

Hazard Statements

May damage the unborn child
Causes damage to organs through prolonged or repeated exposure
Fatal if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

Obtain special instructions before use
Do not handle until all safety precautions have been read and understood
Use personal protective equipment as required
Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Do not get in eyes, on skin, or on clothing
Do not breathe dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Wear respiratory protection

Response

IF exposed or concerned: Get medical attention/advice

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Immediately call a POISON CENTER or doctor/physician

Skin

Immediately call a POISON CENTER or doctor/physician
IF ON SKIN: Gently wash with plenty of soap and water
Remove/Take off immediately all contaminated clothing
Wash contaminated clothing before reuse

Ingestion

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

Storage

Store locked up
Store in a well-ventilated place. Keep container tightly closed

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

Toxic to aquatic life with long lasting effects
WARNING. Reproductive Harm - <https://www.p65warnings.ca.gov/>.

3. Composition/Information on Ingredients

Component	CAS No	Weight %
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	81-81-2	>95

4. First-aid measures

General Advice

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

Eye Contact

In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.

Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.
Most important symptoms and effects	None reasonably foreseeable.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam.
Unsuitable Extinguishing Media	No information available
Flash Point	No information available
Method -	No information available
Autoignition Temperature	Not applicable
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂).

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

NFPA

Health	Flammability	Instability	Physical hazards
4	1	0	N/A

6. Accidental release measures

Personal Precautions	Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas.
Environmental Precautions	Do not flush into surface water or sanitary sewer system.
Methods for Containment and Clean Up	Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

7. Handling and storage

Handling	Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid dust formation. Use only under a chemical fume hood. Do not breathe (dust, vapor, mist, gas). Do not ingest. If swallowed then seek immediate medical assistance.
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Storage. Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Strong oxidizing agents. Strong acids. Strong bases.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH	Mexico OEL (TWA)
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	TWA: 0.01 mg/m ³ Skin	(Vacated) TWA: 0.1 mg/m ³ TWA: 0.1 mg/m ³	IDLH: 100 mg/m ³ TWA: 0.1 mg/m ³	TWA: 0.1 mg/m ³

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH IDLH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures Ensure adequate ventilation, especially in confined areas.

Personal Protective Equipment

Eye/face Protection	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure.
Respiratory Protection	Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Powder Solid
Appearance	White
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	162 - 164 °C / 323.6 - 327.2 °F
Boiling Point/Range	No information available
Flash Point	No information available
Evaporation Rate	Not applicable
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	Not applicable
Specific Gravity	No information available
Solubility	Insoluble in water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	Not applicable
Decomposition Temperature	No information available
Viscosity	Not applicable
Molecular Formula	C ₁₉ H ₁₆ O ₄
Molecular Weight	308.34

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under recommended storage conditions.
Conditions to Avoid	Incompatible products. Avoid dust formation.
Incompatible Materials	Strong oxidizing agents, Strong acids, Strong bases
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	LD50 = 1600 µg/kg (Rat)	LD50 = 1400 mg/kg (Rat)	Not listed

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	81-81-2	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects May cause harm to the unborn child.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure None known

STOT - repeated exposure Blood

Aspiration hazard No information available

Symptoms / effects, both acute and delayed No information available

Endocrine Disruptor Information No information available

Other Adverse Effects .

12. Ecological information

Ecotoxicity

The product contains following substances which are hazardous for the environment. Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Persistence and Degradability	Persistence is unlikely Insoluble in water
Bioaccumulation/ Accumulation	No information available.
Mobility	Is not likely mobile in the environment due its low water solubility.

13. Disposal considerations

Waste Disposal Methods	Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.
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Component	RCRA - U Series Wastes	RCRA - P Series Wastes
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin - 81-81-2	U248	when present at concentrations >0.3%

14. Transport information

DOT

UN-No	UN2811
Proper Shipping Name	Toxic solid, organic, n.o.s.
Technical Name	4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin
Hazard Class	6.1
Packing Group	I

TDG

UN-No	UN2811
Proper Shipping Name	Toxic solid, organic, n.o.s.
Hazard Class	6.1
Packing Group	I

IATA

UN-No	UN2811
Proper Shipping Name	Toxic solid, organic, n.o.s.
Hazard Class	6.1
Packing Group	I

IMDG/IMO

UN-No	UN2811
Proper Shipping Name	Toxic solid, organic, n.o.s.
Hazard Class	6.1
Packing Group	I

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
4-Hydroxy-3-(3-oxo-1-phenylbutyl) coumarin	81-81-2	X	ACTIVE	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
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4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	81-81-2	X	-	201-377-6	X	X	X	-	X	KE-20784
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KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations

SARA 313

Component	CAS No	Weight %	SARA 313 - Threshold Values %
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	81-81-2	>95	1.0

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA Not applicable

Component	Hazardous Substances RQs	CERCLA EHS RQs
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	100 lb	100 lb

California Proposition 65 This product contains the following Proposition 65 chemicals.

Component	CAS No	California Prop. 65	Prop 65 NSRL	Category
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	81-81-2	Developmental	-	Developmental

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	X	X	X	-	-

U.S. Department of Transportation

Reportable Quantity (RQ): Y
 DOT Marine Pollutant Y
 DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH

Component	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	-	Use restricted. See item 30. (see link for restriction details) Use restricted. See item 75. (see link for restriction details)	-

<https://echa.europa.eu/substances-restricted-under-reach>

Safety, health and environmental regulations/legislation specific for the substance or mixture

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	81-81-2	Not applicable	Not applicable	Not applicable	Not applicable

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	81-81-2	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

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Creation Date 13-Sep-2013

Revision Date 28-Dec-2021

Print Date 28-Dec-2021

Revision Summary This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS