

Creation Date 13-Sep-2013

Revision Date 06-Oct-2023

Revision Number 6

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description:	4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin
Cat No. :	454680000; 454680100
Synonyms	Coumafene ; Warfarin
Index No	607-056-00-0
CAS No	81-81-2
EC No	201-377-6
Molecular Formula	C19 H16 O4

1.2. Relevant identified uses of the substance or mixture and uses advised against

Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

1.3. Details of the supplier of the safety data sheet

Company

UK entity/business name
Fisher Scientific UK
Bishop Meadow Road,
Loughborough, Leicestershire LE11 5RG,
United Kingdom

EU entity/business name
Thermo Fisher Scientific
Janssen Pharmaceuticaaan 3a, 2440 Geel,
Belgium

E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **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

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

Physical hazards

Based on available data, the classification criteria are not met

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Health hazards

Acute oral toxicity
Acute dermal toxicity
Acute Inhalation Toxicity - Dusts and Mists
Reproductive Toxicity
Specific target organ toxicity - (repeated exposure)

Category 1 (H300)
Category 1 (H310)
Category 1 (H330)
Category 1A (H360D)
Category 1 (H372)

Environmental hazards

Chronic aquatic toxicity

Category 2 (H411)

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

H360D - May damage the unborn child
H372 - Causes damage to organs through prolonged or repeated exposure
H411 - Toxic to aquatic life with long lasting effects
H300 + H310 + H330 - Fatal if swallowed, in contact with skin or if inhaled

Precautionary Statements

P330 - Rinse mouth
P302 + P350 - IF ON SKIN: Gently wash with plenty of soap and water
P310 - Immediately call a POISON CENTER or doctor/physician
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P280 - Wear protective gloves/protective clothing/eye protection/face protection

Additional EU labelling

Restricted to professional users

2.3. Other hazards

Toxic to terrestrial vertebrates
This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	81-81-2	EEC No. 201-377-6	>95	Acute Tox. 1 (H300)

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				Acute Tox. 1 (H310) Acute Tox. 1 (H330) Repr. 1A (H360D) STOT RE 1 (H372) Aquatic Chronic 2 (H411)
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Component	Specific concentration limits (SCL's)	M-Factor	Component notes
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	STOT RE 1 (H372) :: C>=0.5% Repr. 1A (H360D) :: C>=0.003% STOT RE 2 (H373) :: 0.05%<=C<0.5%	-	-

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of 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.
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.
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.
Self-Protection of the First Aider	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

4.2. Most important symptoms and effects, both acute and delayed

None reasonably foreseeable.

4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician	Treat symptomatically.
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SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam.

Extinguishing media which must not be used for safety reasons

No information available.

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5.2. Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors.

Hazardous Combustion Products

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

5.3. Advice 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.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

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.

6.2. Environmental precautions

Do not flush into surface water or sanitary sewer system.

6.3. Methods and material for containment and cleaning up

Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe 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.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

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

Technical Rules for Hazardous Substances (TRGS) 510 Class 6.1A
Storage Class (LGK) (Germany)

7.3. Specific end use(s)

Use in laboratories

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SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

List source(s): IRE - 2021 Code of Practice for the Chemical Agents Regulations, Schedule 1. Published by the Health and Safety Authority

Component	The United Kingdom	European Union	Ireland
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin			TWA: 0.1 mg/m ³ 8 hr. STEL: 0.3 mg/m ³ 15 min

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

Predicted No Effect Concentration (PNEC)

No information available.

8.2. Exposure controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

Eye Protection

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers	-	EN 374	(minimum requirement)
Nitrile rubber	recommendations			
Neoprene				
PVC				

Skin and body protection

Long sleeved clothing.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

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	To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly
Large scale/emergency use	Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced Recommended Filter type: Particulates filter conforming to EN 143
Small scale/Laboratory use	Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. Recommended half mask:- Particle filtering: EN149:2001 When RPE is used a face piece Fit Test should be conducted
Environmental exposure controls	Prevent product from entering drains. Do not allow material to contaminate ground water system.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Powder Solid	
Appearance	White	
Odor	No information available	
Odor Threshold	No data available	
Melting Point/Range	162 - 164 °C / 323.6 - 327.2 °F	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flammability (liquid)	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Flash Point	No information available	Method - No information available
Autoignition Temperature	Not applicable	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	Not applicable	Solid
Water Solubility	Insoluble	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	No data available	
Bulk Density	No data available	
Vapor Density	Not applicable	Solid
Particle characteristics	No data available	

9.2. Other information

Molecular Formula	C19 H16 O4
Molecular Weight	308.34
Evaporation Rate	Not applicable - Solid

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

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Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

Hazardous Polymerization No information available.
Hazardous Reactions None under normal processing.

10.4. Conditions to avoid

Incompatible products. Avoid dust formation.

10.5. Incompatible materials

Strong oxidizing agents. Strong acids. Strong bases.

10.6. Hazardous decomposition products

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

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

(a) acute toxicity;
Oral Category 1
Dermal Category 1
Inhalation Category 1

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)	-

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;
Respiratory No data available
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity;
There are no known carcinogenic chemicals in this product

(g) reproductive toxicity;
Reproductive Effects Category 1A
May cause harm to the unborn child.

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; Category 1
Target Organs Blood, Central Vascular System (CVS).

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(j) aspiration hazard; Not applicable
Solid

Other Adverse Effects

Symptoms / effects, both acute and delayed No information available.

11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects 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.

12.2. Persistence and degradability

Persistence Persistence is unlikely, Insoluble in water.
Degradation in sewage treatment plant Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

12.3. Bioaccumulative potential May have some potential to bioaccumulate

Component	log Pow	Bioconcentration factor (BCF)
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin		1.7

12.4. Mobility in soil Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility.

12.5. Results of PBT and vPvB assessment No data available for assessment.

12.6. Endocrine disrupting properties

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

Persistent Organic Pollutant This product does not contain any known or suspected substance
Ozone Depletion Potential This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues/Unused Products Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

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Contaminated Packaging	Dispose of this container to hazardous or special waste collection point.
European Waste Catalogue (EWC)	According to the European Waste Catalog, Waste Codes are not product specific, but application specific.
Other Information	Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Do not let this chemical enter the environment.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number	UN2811
14.2. UN proper shipping name	Toxic solid, organic, n.o.s.
Technical Shipping Name	4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin
14.3. Transport hazard class(es)	6.1
14.4. Packing group	I

ADR

14.1. UN number	UN2811
14.2. UN proper shipping name	Toxic solid, organic, n.o.s.
Technical Shipping Name	4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin
14.3. Transport hazard class(es)	6.1
14.4. Packing group	I

IATA

14.1. UN number	UN2811
14.2. UN proper shipping name	Toxic solid, organic, n.o.s.
Technical Shipping Name	4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin
14.3. Transport hazard class(es)	6.1
14.4. Packing group	I

14.5. Environmental hazards	Dangerous for the environment Product is a marine pollutant according to the criteria set by IMDG/IMO
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14.6. Special precautions for user	No special precautions required.
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14.7. Maritime transport in bulk according to IMO instruments	Not applicable, packaged goods
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SECTION 15: REGULATORY INFORMATION

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

International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
4-Hydroxy-3-(3-oxo-1-phenylbutyl)	81-81-2	201-377-6	-	-	X	X	KE-20784	X	X

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coumarin								
Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	81-81-2	X	ACTIVE	X	-	-	X	X

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Authorisation/Restrictions according to EU REACH

Component	CAS No	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	81-81-2	-	Use restricted. See item 30. (see link for restriction details) Use restricted. See item 75. (see link for restriction details)	-

REACH links

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

Seveso III Directive (2012/18/EC)

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
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin	81-81-2	Not applicable	Not applicable

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Component	ANNEX I - PART 1 List of chemicals subject to export notification procedure (referred to in Article 8)	ANNEX I - PART 2 List of chemicals qualifying for PIC notification (referred to in Article 11)	ANNEX I - PART 3 List of chemicals subject to the PIC procedure (referred to in Articles 13 and 14)
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin 81-81-2 (>95)	p(1) — pesticide in the group of plant protection products b — ban (for the category or categories concerned) b — ban (for the category or categories concerned)	-	-

<https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A32012R0649&qid=1604065742303>.

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

Take note of Directive 94/33/EC on the protection of young people at work

Take note of Dir 92/85/EC on the protection of pregnant and breastfeeding women at work

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National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification Water endangering class = 3 (self classification)

Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin 81-81-2 (>95)	Prohibited and Restricted Substances		

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

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

H300 - Fatal if swallowed

H310 - Fatal in contact with skin

H330 - Fatal if inhaled

H360D - May damage the unborn child

H372 - Causes damage to organs through prolonged or repeated exposure

H411 - Toxic to aquatic life with long lasting effects

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

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Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Creation Date	13-Sep-2013
Revision Date	06-Oct-2023
Revision Summary	Not applicable.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

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 Safety Data Sheet