# SAFETY DATA SHEET

**Creation Date** 13-Sep-2013 **Revision Date** 25-Sep-2017 **Revision Number** 3

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

### 1.1. Product identification

| | |
|---|---|
| **Product Description:** | **4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin** |
| **Cat No. :** | **454680000; 454680100** |
| **Synonyms** | Coumafene ; Warfarin |
| **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** | Acros Organics BVBA<br>Janssen Pharmaceuticalaan 3a<br>2440 Geel, Belgium |
| **E-mail address** | begel.sdsdesk@thermofisher.com |

### 1.4. 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

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

**CLP Classification - Regulation (EC) No 1272/2008**

**Physical hazards**

Based on available data, the classification criteria are not met

**Health hazards**

| | |
|---|---|
| Acute oral toxicity | Category 1 (H300) |
| Acute dermal toxicity | Category 1 (H310) |
| Acute Inhalation Toxicity - Dusts and Mists | Category 1 (H330) |
| Reproductive Toxicity | Category 1A (H360D) |
| Specific target organ toxicity - (repeated exposure) | Category 1 (H372) |

**Environmental hazards**

| | |
|---|---|
| Chronic aquatic toxicity | Category 2 (H411) |

### 2.2. Label elements

**Signal Word** **Danger**

**Hazard Statements**

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

**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 to fresh air and keep at rest in a position comfortable for breathing
P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection

**Additional EU labelling**

Restricted to professional users

### 2.3. Other hazards

No information available

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

| Component | CAS-No | EC-No. | Weight % | CLP Classification - Regulation (EC) No 1272/2008 |
|---|---|---|---|---|
| 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin | 81-81-2 | EEC No. 201-377-6 | >95 | Acute Tox. 1 (H300)<br>Acute Tox. 1 (H310)<br>Acute Tox. 1 (H330)<br>Repr. 1A (H360D)<br>STOT RE 1 (H372)<br>Aquatic Chronic 2 (H411) |

*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** Move 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.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

**Suitable Extinguishing Media**
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

**Extinguishing media which must not be used for safety reasons**
No information available.

### 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 ($CO_2$).

### 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. 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 or vacuum up spillage and collect in suitable container 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. Do not get in eyes, on skin, or on clothing. Avoid dust formation. Use only under a chemical fume hood. Do not breathe vapors/dust. Do not ingest.

**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 before re-use. Wash hands before breaks and at the end of workday.

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

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

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

**Exposure limits**
List source(s): **IRE -** 2010 Code of Practice for the Safety, Health and Welfare at Work (Chemical Agents) Regulations 2001. Published by the Health and Safety Authority.

| Component | European Union | The United Kingdom | France | Belgium | Spain |
|---|---|---|---|---|---|
| 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin | | | TWA / VME: 0.1 mg/m³ (8 heures). | TWA: 0.1 mg/m³ 8 uren | TWA / VLA-ED: 0.1 mg/m³ (8 horas) |

| Component | Italy | Germany | Portugal | The Netherlands | Finland |
|---|---|---|---|---|---|
| 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin | | TWA: 0.0016 ppm (8 Stunden). AGW - exposure factor 8<br>TWA: 0.02 mg/m³ (8 Stunden). AGW - exposure factor 8<br>TWA: 0.0016 ppm (8 Stunden). MAK can occur as vapor and aerosol at the same time<br>TWA: 0.02 mg/m³ (8 Stunden). MAK can | TWA: 0.1 mg/m³ 8 horas | | TWA: 0.1 mg/m³ 8 tunteina<br>STEL: 0.3 mg/m³ 15 minuutteina |

| | | | | | |
|---|---|---|---|---|---|
| | | occur as vapor and aerosol at the same time<br>Höhepunkt: 0.0128 ppm<br>Höhepunkt: 0.16 mg/m³<br>Haut | | | |

| Component | Austria | Denmark | Switzerland | Poland | Norway |
|---|---|---|---|---|---|
| 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin | MAK-KZW: 0.5 mg/m³ 15 Minuten<br>MAK-TMW: 0.1 mg/m³ 8 Stunden | TWA: 0.1 mg/m³ 8 timer | Haut/Peau<br>STEL: 0.16 mg/m³ 15 Minuten<br>STEL: 0.0128 ppm 15 Minuten<br>TWA: 0.0016 ppm 8 Stunden<br>TWA: 0.02 mg/m³ 8 Stunden | | TWA: 0.1 mg/m³ 8 timer<br>STEL: 0.3 mg/m³ 15 minutter. value calculated |

| Component | Bulgaria | Croatia | Ireland | Cyprus | Czech Republic |
|---|---|---|---|---|---|
| 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin | | TWA-GVI: 0.5 mg/m³ 8 satima.<br>STEL-KGVI: 1.5 mg/m³ 15 minutama. | TWA: 0.1 mg/m³ 8 hr.<br>STEL: 0.3 mg/m³ 15 min | | |

| Component | Estonia | Gibraltar | Greece | Hungary | Iceland |
|---|---|---|---|---|---|
| 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin | | | TWA: 0.5 mg/m³ | | TWA: 0.1 mg/m³ 8 klukkustundum.<br>Ceiling: 0.2 mg/m³ |

| Component | Latvia | Lithuania | Luxembourg | Malta | Romania |
|---|---|---|---|---|---|
| 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin | TWA: 0.001 mg/m³ | | | | Skin notation<br>TWA: 0.1 mg/m³ 8 ore<br>STEL: 0.3 mg/m³ 15 minute |

| Component | Russia | Slovak Republic | Slovenia | Sweden | Turkey |
|---|---|---|---|---|---|
| 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin | MAC: 0.001 mg/m³ | | TWA: 0.5 mg/m³ 8 urah inhalable fraction<br>STEL: 2 mg/m³ 15 minutah inhalable fraction | | |

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

**Monitoring methods**
BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.
MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

**Derived No Effect Level (DNEL)** No information available

| Route of exposure | Acute effects (local) | Acute effects (systemic) | Chronic effects (local) | Chronic effects (systemic) |
|---|---|---|---|---|
| **Oral** | | | | |
| **Dermal** | | | | |
| **Inhalation** | | | | |

**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** Safety glasses with side-shields (European standard - EN 166)

**Hand Protection** Protective gloves

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

**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 compatability, 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.
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

**Appearance** White
**Physical State** Powder Solid

**Odor** No information available
**Odor Threshold** No data available
**pH** No information available
**Melting Point/Range** 162 - 164 °C / 323.6 - 327.2 °F
**Softening Point** No data available
**Boiling Point/Range** No information available

| | | |
|---|---|---|
| **Flash Point** | No information available | **Method -** No information available |
| **Evaporation Rate** | Not applicable | Solid |
| **Flammability (solid,gas)** | No information available | |
| **Explosion Limits** | No data available | |
| **Vapor Pressure** | No data available | |
| **Vapor Density** | Not applicable | Solid |
| **Specific Gravity / Density** | No data available | |
| **Bulk Density** | No data available | |
| **Water Solubility** | Insoluble | |
| **Solubility in other solvents** | No information available | |
| **Partition Coefficient (n-octanol/water)** | | |
| **Autoignition Temperature** | Not applicable | |
| **Decomposition Temperature** | No data available | |
| **Viscosity** | Not applicable | Solid |
| **Explosive Properties** | No information available | |
| **Oxidizing Properties** | No information available | |

**9.2. Other information**

| | |
|---|---|
| **Molecular Formula** | C19 H16 O4 |
| **Molecular Weight** | 308.34 |

## SECTION 10: STABILITY AND REACTIVITY

**10.1. Reactivity**

None known, based on information available

**10.2. Chemical stability**

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 ($CO_2$).

## SECTION 11: TOXICOLOGICAL INFORMATION

**11.1. Information on toxicological effects**

**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 = 1.6 mg/kg ( Rat )<br>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;** Category 1A
**Reproductive Effects** 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).

**(j) aspiration hazard;** Not applicable
Solid

**Other Adverse Effects**

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

## 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

**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. Other adverse effects**

| | |
|---|---|
| **Endocrine Disruptor Information** | This product does not contain any known or suspected endocrine disruptors |
| **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. |
| **Contaminated Packaging** | Dispose of this container to hazardous or special waste collection point. |
| **European Waste Catalogue (EWC)** | According to the European Waste Catalogue, Waste Codes are not product specific, but application specific. |
| **Other Information** | Do not dispose of waste into 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

**14.6. Special precautions for user** No special precautions required

**14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code** Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

**International Inventories** X = listed

| Component | EINECS | ELINCS | NLP | TSCA | DSL | NDSL | PICCS | ENCS | IECSC | AICS | KECL |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin | 201-377-6 | - | | X | X | - | X | X | X | X | X |

| 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 *http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=CELEX:32006R1907:EN:NOT* for restriction details) | |

**National Regulations**

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

### 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/NDSL** - 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
**PNEC** - Predicted No Effect Concentration
**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
**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 Compounds

**Key literature references and sources for data**
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** | 25-Sep-2017 |
| **Revision Summary** | SDS sections updated: 2, 3, 12, 16. |



## End of Safety Data Sheet