

Chemical Safety Data Sheet MSDS / SDS

Coumarin

Revision Date:2024-05-18 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier

Product name : Coumarin
CBnumber : CB3112168
CAS : 91-64-5
EINECS Number : 202-086-7
Synonyms : coumarin,COUMARINE

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification

Classification of the substance or mixture

Acute toxicity - Category 4, Oral
Skin sensitization, Category 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

Label elements**Pictogram(s)**

☐

Signal word : Danger

Hazard statement(s)

H301 Toxic if swallowed
H351 Suspected of causing cancer

Precautionary statement(s)

P201 Obtain special instructions before use.
P264 Wash hands thoroughly after handling.
P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

P308+P313 IF exposed or concerned: Get medical advice/attention.

P405 Store locked up.

P501 Dispose of contents/container to.....

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P272 Contaminated work clothing should not be allowed out of the workplace.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P273 Avoid release to the environment.

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P333+P317 If skin irritation or rash occurs: Get medical help.

P321 Specific treatment (see ... on this label).

P362+P364 Take off contaminated clothing and wash it before reuse.

Storage

none

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

| | |
|--------------|-----------------------|
| Product name | : Coumarin |
| Synonyms | : coumarin, COUMARINE |
| CAS | : 91-64-5 |
| EC number | : 202-086-7 |
| MF | : C9H6O2 |
| MW | : 146.14 |

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Refer for medical attention .

Most important symptoms and effects, both acute and delayed

SYMPTOMS: Exposure to this compound may cause narcosis. It may also cause irritation and liver damage. (NTP, 1992)

Indication of any immediate medical attention and special treatment needed

Absorption, Distribution and Excretion

A species difference has been reported for the excretion of an oral dose of (14)C-coumarin. Within 4 days rats excreted 47% of the label in the urine and 39% in the feces, whereas rabbits excreted 92% in the urine and negligible amount in the feces.

SECTION 5: Firefighting measures

Extinguishing media

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. A water spray may also be used. (NTP, 1992)

Specific Hazards Arising from the Chemical

This chemical is combustible. (NTP, 1992)

Advice for firefighters

Use water spray, foam, powder, carbon dioxide.

NFPA 704



■ HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

■ FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N₂](#))

- SPEC.
 - HAZ.
-

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Separated from food and feedstuffs.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures

Eye/face protection

Wear face shield.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

| | |
|--|---|
| Physical state | Crystals or Crystalline Powder |
| Colour | White |
| Odour | Pleasant, fragrant odor resembling that of vanilla beans. |
| Melting point/freezing point | Ca. 69 °C. Atm. press.:Ca. 1 atm. |
| Boiling point or initial boiling point and boiling range | Ca. 298 °C. Atm. press.:Ca. 1 atm. |
| Flammability | Combustible. |
| Lower and upper explosion limit/flammability limit | no data available |
| Flash point | 162 °C. Atm. press.:1 atm. |
| Auto-ignition temperature | no data available |
| Decomposition temperature | no data available |
| pH | no data available |
| Kinematic viscosity | no data available |
| Solubility | 1.7g/l |
| Partition coefficient n-octanol/water | log Pow = 1.39. Temperature:25 °C. |
| Vapour pressure | 0.01 mm Hg (47 °C) |
| Density and/or relative density | Ca. 0.935 kg/m3. Temperature:20 °C. |
| Relative vapour density | no data available |
| Particle characteristics | no data available |

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

Converted to a dimer on long exposure to light.

Possibility of hazardous reactions

SLIGHT, WHEN EXPOSED TO HEAT OR FLAME.COUMARIN is sensitive to exposure to light. It is also sensitive to heat. This chemical is
Chemical Book

incompatible with strong acids, strong bases and oxidizers. It is hydrolyzed by hot concentrated alkalis. It can be halogenated, nitrated and hydrogenated (in the presence of catalysts). (NTP, 1992)

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 - rat (male/female) - 293 mg/kg bw.
- Inhalation: LC50 - rat (male/female) - 293 mg/kg.
- Dermal: LD50 - rat (male/female) - 293 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

Evaluation: No epidemiological data relevant to the carcinogenicity of coumarin were available. There is limited evidence in experimental animals for the carcinogenicity of coumarin. Overall evaluation: Coumarin is not classifiable as to its carcinogenicity to humans (Group 3).

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the skin.

STOT-repeated exposure

This substance is possibly carcinogenic to humans.

Aspiration hazard

Evaporation at 20°C is negligible; a nuisance-causing concentration of airborne particles can, however, be reached quickly.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - 2.94 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia sp. - 8.012 mg/L - 48 h.

Toxicity to algae: EC50 - 1.452 mg/L - 96 h.

Toxicity to microorganisms: IC50 - activated sludge - 640 mg/L - 3 h. Remarks:Respiration rate.

Persistence and degradability

AEROBIC: In a 5 day biodegradation screening test using an activated sludge inoculum, 29.5% of coumarin was mineralized(1). Coumarin, present at 100 mg/l, reached 100% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/l and the Japanese MITI test(2). Coumarin degraded after one week in soil contaminated with diesel fuel which was then incubated in the dark at ambient temperature for 25 weeks(3).

Bioaccumulative potential

The BCF in golden orfe was <10 after 3 days exposure(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC). The BCF of coumarin in green algae (*Chlorella* sp.) after exposure to 50 ug/l of coumarin for 24 hr was 42(1).

Mobility in soil

The Koc of coumarin is estimated as 140(SRC), using a log Kow of 1.39(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that coumarin is expected to have high mobility in soil.

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN2811 (For reference only, please check.)

IMDG: UN2811 (For reference only, please check.)

IATA: UN2811 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)

IMDG: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)

IATA: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

PICCS

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Disclaimer:

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