

## Chemical Safety Data Sheet MSDS / SDS

**2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-(3,4,5-trihydroxy-6-methyl-oxa n-2-yl)oxy-chroman-4-one**

Revision Date:2026-03-22 Revision Number:1

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

Product name : 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-(3,4,5-trihydroxy-6-methyl-oxa n-2-yl)oxy-chroman-4-one  
CBnumber : CB41261031  
CAS : 54141-72-9  
Synonyms : Nsc245342;Neoisoastilbin

**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 : 010-86108875

**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

**Precautionary statements**

P501 Dispose of contents/container to....

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

P264 Wash skin thoroughly after handling.

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

P302+P352 IF ON SKIN: wash with plenty of soap and water.

P337+P313 IF eye irritation persists: Get medical advice/attention.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

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P332+P313 IF SKIN irritation occurs: Get medical advice/attention.

**Hazard statements**

H302 Harmful if swallowed  
H315 Causes skin irritation  
H319 Causes serious eye irritation

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## SECTION 3: Composition/information on ingredients

### Substance

Product name : 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-(3,4,5-trihydroxy-6-methyl-oxa n-2-yl)oxy-chroman-4-one  
Synonyms : Neisoastilbin,(2S,3R)-Astilbin  
CAS : 54141-72-9  
MF : C<sub>21</sub>H<sub>22</sub>O<sub>11</sub>  
MW : 450.39

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## SECTION 4: First aid measures

### 4.1 Description of first aid measures

#### Eye contact

Remove any contact lenses, locate eye-wash station, and flush eyes immediately with large amounts of water. Separate eyelids with fingers to ensure adequate flushing. Promptly call a physician.

#### Skin contact

Rinse skin thoroughly with large amounts of water. Remove contaminated clothing and shoes and call a physician.

#### Inhalation

Immediately relocate self or casualty to fresh air. If breathing is difficult, give cardiopulmonary resuscitation (CPR). Avoid mouth- to-mouth resuscitation.

#### Ingestion

Wash out mouth with water; Do NOT induce vomiting; call 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).

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

Treat symptomatically.

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, dry chemical, foam, and carbon dioxide fire extinguisher.

### 5.2 Special hazards arising from the substance or mixture

During combustion, may emit irritant fumes.

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus and protective clothing.

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Use full personal protective equipment. Avoid breathing vapors, mist, dust or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

Refer to protective measures listed in sections 8.

### 6.2 Environmental precautions

Try to prevent further leakage or spillage. Keep the product away from drains or water courses.

### 6.3 Methods and materials for containment and cleaning up

Absorb solutions with finely-powdered liquid-binding material (diatomite, universal binders); Decontaminate surfaces and equipment by scrubbing with alcohol; Dispose of contaminated material according to Section 13.

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Avoid inhalation, contact with eyes and skin. Avoid dust and aerosol formation. Use only in areas with appropriate exhaust ventilation.

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

Keep container tightly sealed in cool, well-ventilated area. Keep away from direct sunlight and sources of ignition.

#### Recommended storage temperature

4°C, stored under nitrogen \* In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen)

Shipping at room temperature if less than 2 weeks.

### 7.3 Specific end use(s)

No data available.

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Components with workplace control parameters

This product contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

### Engineering controls

Ensure adequate ventilation. Provide accessible safety shower and eye wash station.

### Personal protective equipment

#### Eye protection

Safety goggles with side-shields.

#### Hand protection

Protective gloves.

#### Skin and body protection

Impervious clothing.

#### Respiratory protection

Suitable respirator.

#### Environmental exposure controls

Keep the product away from drains, water courses or the soil. Clean spillages in a safe way as soon as possible.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	Solid
Odor	No data available
Odor threshold	No data available
pH	No data available
Melting/freezing point	168-169°C
Boiling point/range	801.1±65.0 °C(Predicted)
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapor pressure	No data available
Vapor density	No data available
Relative density	1.74±0.1 g/cm <sup>3</sup> (Predicted)
Water Solubility	No data available
Partition coefficient	No data available
Auto-ignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available
Physical state	Solid
Colour	Off-white to light yellow

### 9.2 Other safety information

No data available.

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## SECTION 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 acids/alkalis, strong oxidising/reducing agents.

### 10.6 Hazardous decomposition products

Under fire conditions, may decompose and emit toxic fumes.

Other decomposition products - no data available.

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Classified based on available data. For more details, see section 2

#### Skin corrosion/irritation

Classified based on available data. For more details, see section 2

#### Serious eye damage/irritation

Classified based on available data. For more details, see section 2

#### Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

#### Germ cell mutagenicity

Classified based on available data. For more details, see section 2

#### Carcinogenicity

##### IARC

No component of this product present at a level equal to or greater than 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

##### ACGIH

No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by ACGIH.

##### NTP

No component of this product present at a level equal to or greater than 0.1% is identified as a anticipated or confirmed carcinogen by NTP.

#### **OSHA**

No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by OSHA.

#### **Reproductive toxicity**

Classified based on available data. For more details, see section 2

#### **Specific target organ toxicity - single exposure**

Classified based on available data. For more details, see section 2

#### **Specific target organ toxicity - repeated exposure**

Classified based on available data. For more details, see section 2

#### **Aspiration hazard**

Classified based on available data. For more details, see section 2

#### **Additional information**

This information is based on our current knowledge. However the chemical, physical, and toxicological properties have not been completely investigated.

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## SECTION 12: Ecological information

### **12.1 Toxicity**

No data available.

### **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 unavailable as chemical safety assessment not required or not conducted.

### **12.6 Other adverse effects**

No data available.

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## SECTION 13: Disposal considerations

### **13.1 Waste treatment methods**

#### **Product**

Dispose substance in accordance with prevailing country, federal, state and local regulations.

#### **Contaminated packaging**

Conduct recycling or disposal in accordance with prevailing country, federal, state and local regulations.

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## SECTION 14: Transport information

### DOT (US)

#### Proper shipping name

Not dangerous goods

#### UN number

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#### Class

-

#### Packing group

-

### IMDG

#### Proper shipping name

Not dangerous goods

#### UN number

-

#### Class

-

#### Packing group

-

### IATA

#### Proper shipping name

Not dangerous goods

#### UN number

-

#### Class

-

#### Packing group

-

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## SECTION 15: Regulatory information

### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### SARA 311/312 Hazards

No SARA Hazards.

### **Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

### **Pennsylvania Right To Know Components**

No components are subject to the Pennsylvania Right to Know Act.

### **New Jersey Right To Know Components**

No components are subject to the New Jersey Right to Know Act.

### **California Prop. 65 Components**

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

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## **SECTION 16: Other information**

### **Abbreviations and acronyms**

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

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

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

#### **Disclaimer:**

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.